

Computing the Flow of Light

NONSTANDARD FDTD METHODOLOGIES
FOR PHOTONICS DESIGN

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Preface

People often speak of *the* finite difference time domain (FDTD) method, as if there were only one such method, formulated long ago by wise sages and fixed for all time. This is not so. FDTD is a topic of active research, and its methodology is constantly evolving. FDTD and FDTD-like methods can be used to solve a wide variety of problems, including—but not limited to—the wave equation, Maxwell’s equations, and the Schrödinger equation.

FDTD is particularly useful for investigating time-dependent phenomena. As the name suggests, the time evolution of a system is computed at discrete time steps, and periodic visualizations can show its time evolution—information that is not available in a frequency domain technique. This yields useful physical insights into transient processes as well as an intuitive feel for what is happening; often, one can see at a glance if something is wrong with a calculation—saving not only computer time, but more importantly, human time.

In essence, *an* FDTD algorithm is derived from *a* difference equation model of the differential equation to be solved by replacing the derivatives with finite difference (FD) expressions. (We use indefinite articles to indicate that there can be more than one FD model and more than one FDTD algorithm.) As we shall demonstrate in this book, the accuracy and stability of FDTD algorithms can be greatly improved by using what are called *nonstandard* FD models on which nonstandard FDTD is based.

High-precision FDTD is the primary—but not the only—subject of this book. Although the basic FDTD algorithm is simple, you will encounter many ‘devils in the details’ when you actually try to use it to solve a problem. Throughout this book we address these devilish details.

Green’s functions, although an elegant analytical construct, are of limited practical use to solve differential equations because they can be difficult to find, but the discrete Green’s function (DGF) of a difference equation model of a differential equation can be found using FDTD. The DGF methodology is a useful alternative to conventional FDTD for certain problems.

Besides introducing useful new methodologies, we have written this book to give our readers new insights, along with the analytical background necessary to develop their own methodologies to solve new problems on the leading edges of photonics and electromagnetics research. We explain not only how FDTD works, but why it works. We delve into the details of a few analytical solutions against which the numerical solutions can be compared to validate FDTD algorithms and to elucidate their limitations.

We make no attempt to be encyclopedic; rather, we delve deeply (devils in the details) into a few of the most important and basic methodologies. We hope that our readers can use this book to write their own working programs and improve on our methods, and that they will share what they have learned with the community.

Our experience in solving real-life applications with FDTD has taught us that there are two distinct communities: those who see FDTD from the algorithmic–computational point of view and those who see themselves primarily as users of black-box software. We believe that FDTD simulations must be guided by an understanding of Maxwell’s equations and how these equations incorporate material properties. This premise is an important focus of this book. Through the simulation examples presented, we have attempted to show that FDTD and related techniques can be very useful in solving practical problems.

Summary of the Contents

- **Chapter 1** introduces FD expressions and develops the notation that is used throughout this book. The appendices give some supplementary advanced topics.
- **Chapter 2** introduces algorithms in general. We analyze a few example algorithms in detail and discuss their accuracy and numerical stability. In the appendices we introduce additional advanced topics. Working programs illustrate some of the main ideas.
- **Chapter 3** develops the basic concepts of the FDTD methodology using the simple harmonic oscillator as a vehicle. We then introduce the nonstandard FDTD methodology. We go on to develop analytic solutions for both the differential equations and their corresponding difference equations using Green’s functions. In the appendices we review some basic mathematical concepts and derive Green’s functions for differential and difference equations. We also analyze the accuracy and stability of a few simple FDTD algorithms.
- **Chapters 4–7** present FDTD for the wave equation. Following a strategy of stepwise increasing complexity, we start with the one-dimensional wave equation and develop the machinery needed to solve useful problems using FDTD. The appendices contain advanced

material (Green's function solutions, including the development of a Green's function for the finite difference form of the wave equation) and deal with various devilish details. We then extend these developments to two and three dimensions, and give some working example programs.

- **Chapter 8** provides a brief review of electromagnetic theory.
- **Chapters 9 and 10** present FDTD for Maxwell's equations. We first develop standard and nonstandard FDTD (the Yee algorithm) in one dimension, and then extend the methodology to two and three dimensions. This completes the development of conventional and *nonstandard* FDTD. Working programs illustrate some the main ideas.
- **Chapter 11** provides example problems.
- **Chapters 12–14** present FDTD for the dispersive case and provide example problems in photonics design. We introduce some of our latest research results on how to improve accuracy in the dispersive case. We solve some interesting photonics problems and discuss photonics design for engineering a subwavelength structure to have desired optical properties.

Audience

Our intended audience includes intelligent beginners such as students, experimental scientists who want to model their experiments, practical engineers, and theoretical researchers grappling with problems that cannot be solved analytically.

We introduce our nonstandard FDTD methodology as a useful tool for computational professionals as well as for beginners.

Very few members of the physics community are aware of the wide utility of FDTD methods, and we hope that our book will inform this group.

We include working FDTD programs that bring wave and electromagnetic phenomena to life. Our analytic solutions motivate the study of mathematical physics as a practical tool. Indeed, this book could be useful for teaching a mathematical physics, applied mathematics, or engineering class.

We also hope that advanced practitioners of FDTD can use this book to extend the nonstandard approach to other FDTD methodologies not covered here.

Finally, this book is written for researchers who want to develop new methodologies that go beyond those we have presented.

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May 2017

Chapter 1

Finite Difference Approximations

Let us begin by explaining the “finite difference” (FD) of the finite difference time domain (FDTD) methodology. We review the basic concepts and mathematical properties of different FD expressions, and introduce the basic concepts and the notation to be used throughout this book.

Topics:

- Elementary finite difference expressions
- Nonstandard finite difference expressions
- Computational molecules

1.1 Basic Finite Difference Expressions

There are three elementary FD expressions for the first derivative:

1. The forward FD (FFD) approximation,

$$\begin{aligned} f'(x) &\cong \frac{f(x+h) - f(x)}{h}, \\ &\cong \frac{d_x^f f(x)}{h}, \end{aligned} \tag{1.1}$$

where

$$d_x^f f(x) = f(x+h) - f(x). \tag{1.2}$$

Expanding $f(x+h)$ in a Taylor series, we find the error of the FFD approximation to be

$$\begin{aligned}
 \varepsilon_{\text{FD}} &= \frac{d_x^f f(x)}{h} - f'(x) \\
 &= \frac{1}{2} h f''(x) + \frac{1}{6} h^2 f'''(x).
 \end{aligned} \tag{1.3}$$

2. The backward FD (BFD) approximation,

$$\begin{aligned}
 f'(x) &\cong \frac{f(x) - f(x-h)}{h} \\
 &\cong \frac{d_x^b f(x)}{h},
 \end{aligned} \tag{1.4}$$

where

$$d_x^b f(x) = f(x) - f(x-h). \tag{1.5}$$

Expanding $f(x+h)$, we find that the error of the BFD approximation is

$$\begin{aligned}
 \varepsilon_{\text{BD}} &= \frac{d_x^b f(x)}{h} - f'(x) \\
 &= -\frac{1}{2} h f''(x) + \frac{1}{6} h^2 f'''(x) \cdots
 \end{aligned} \tag{1.6}$$

The forward- and backward-FD approximations are said to be first-order accurate or simply “first-order” because the error is proportional to the first power of h .

3. The central FD (CFD) approximation,

$$\begin{aligned}
 f'(x) &\cong \frac{f(x+h/2) - f(x-h/2)}{h} \\
 &\cong \frac{d_x^c f(x)}{h},
 \end{aligned} \tag{1.7}$$

where

$$d_x^c f(x) = f(x+h/2) - f(x-h/2). \tag{1.8}$$

Expanding $f(x+h/2) - f(x-h/2)$, we find the error of the CFD approximation to be

$$\begin{aligned}
 \varepsilon_{\text{CD}} &= \frac{d_x^c f(x)}{h} - f'(x) \\
 &= \frac{1}{24} h^2 f'''(x) + \cdots;
 \end{aligned} \tag{1.9}$$

thus, the CFD approximation to f' is second-order accurate.

Comparing Eq. (1.3) with Eq. (1.9), one might suppose that $\varepsilon_{CD} < \varepsilon_{FD}$, but this is true only if $h^2 f'''(x)/24 + \cdots < hf''(x)/2 + \cdots$. For example, taking $f(x) = e^{\alpha x}$ with $\alpha > h$, the error of the FFD approximation is actually smaller than that of the CFD approximation.

Accuracy is not the only criterion for the choice of an FD expression in constructing an algorithm. It is essential that the algorithm be *numerically stable* as well as accurate. (See Section 2.4 for an example of how highly accurate FD algorithms can display perverse behavior.)

For future reference we derive the CFD approximation for $f''(x)$:

$$\begin{aligned} f''(x) &\cong \frac{d_x^c}{h} \left[\frac{d_x^c}{h} f(x) \right] \\ &= \frac{(d_x^c)^2}{h^2} f(x) \\ &= \frac{f(x+h) + f(x-h) - 2f(x)}{h^2}, \end{aligned} \quad (1.10)$$

where $(d_x^c)^2 = d_x^c d_x^c$. It is straightforward to show that

$$(d_x^c)^2 f(x) = f(x+h) + f(x-h) - 2f(x). \quad (1.11)$$

Expanding Eq. (1.10) in a Taylor series about x , we find that

$$\frac{(d_x^c)^2}{h^2} f(x) = f''(x) + \frac{1}{12} h^2 f^{(4)}(x) + \cdots; \quad (1.12)$$

thus, the CFD approximation of f'' is second-order accurate.

We shall henceforth refer to the above FD expressions as standard finite difference (S-FD) expressions for reasons that will soon be apparent.

1.1.1 Higher-order finite difference approximations

Retaining only the first two terms of expansion of Eq. (A1.1.12) in Appendix 1, we obtain

$$\begin{aligned} \partial_x f(x) &\cong \frac{1}{h} \left[d_x^c - \frac{1}{24} (d_x^c)^3 \right] f(x) \\ &\cong \frac{1}{h} \left\{ \frac{7}{8} [f(x+h/2) - f(x-h/2)] \right. \\ &\quad \left. - \frac{1}{24} [f(x+3h/2) - f(x-3h/2)] \right\}, \end{aligned} \quad (1.13)$$

where we have used Eq. (A1.2.25b) to expand $(d_x^c)^3 f(x)$. Expanding the right side in a Taylor series, we find that

$$\frac{1}{h} \left[d_x^c - \frac{1}{24} (d_x^c)^3 \right] f(x) = f'(x) - \frac{3}{640} h^4 f^{(5)}(x) + \cdots \quad (1.14)$$

Thus, Eq. (1.14) is a fourth-order FD approximation to f' .

Similarly, the fourth-order approximation for the second derivative is found by retaining the first two terms of expansion Eq. (A1.13) and using Eq. (A1.2.25c) to expand $(d_x^c)^4 f(x)$ to obtain

$$\begin{aligned} \partial_x^2 f(x) &\cong \frac{1}{h^2} \left[(d_x^c)^2 - \frac{1}{12} (d_x^c)^4 \right] f(x) \\ &\cong \frac{1}{h^2} \left\{ \frac{4}{3} [f(x+h) + f(x-h)] \right. \\ &\quad \left. - \frac{1}{12} [f(x+2h) + f(x-2h)] - \frac{5}{2} f(x) \right\}. \end{aligned} \quad (1.15)$$

Expanding the right side of Eq. (1.15) in a Taylor series, we find that

$$\frac{1}{h^2} \left[(d_x^c)^2 - \frac{1}{12} (d_x^c)^4 \right] f(x) = f''(x) - \frac{h^4}{90} f^{(6)}(x) + \cdots; \quad (1.16)$$

hence, Eq. (1.16) is a fourth-order FD approximation to f'' .

1.1.2 Computational molecules

The graphical representation of the difference operators yields useful insights. For example, the central difference operator for the first derivative, $d_x^c f(x) = f(x+h/2) - f(x-h/2)$ in Eq. (1.8), can be represented by the graph in Fig. 1.1. The node position corresponds to the local function value, and its weight in the finite difference expression is indicated. Usually the function value is omitted.

The central difference operator for the second derivative, $(d_x^c)^2 f(x) = f(x+h) - 2f(x) + f(x-h)$ in Eq. (1.11), can be represented as shown in Fig. 1.2.

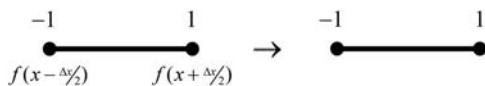


Figure 1.1 Computational molecule for d_x^c .

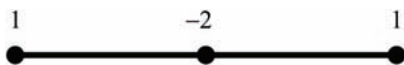


Figure 1.2 Computational molecule for $(d_x^c)^2$.

1.2 Nonstandard Finite Difference Expressions

Besides the forward-, backward-, and central-FD approximations, there is another more general class known as nonstandard finite difference (NS-FD) approximations, which were introduced by Mickens.¹ Using NS-FD expressions, it is sometimes possible to greatly reduce the error of an FD approximation and even to eliminate it.

The most general NS-FD approximation is given by

$$f'(x)|_{x=y} \cong \frac{f(x+h) - a(h)f(x)}{s(h)}, \quad (1.17)$$

where a and s are functions. The central FD approximation is a special case of Eq. (1.17) with $y = x + h/2$, $a = 1$, and $s(h) = h$. For a NS-FD expression to be a valid approximation of the derivative, it must converge to $f'(x)$ in the limit $h \rightarrow 0$:

$$f'(x)|_{x=y} = \lim_{h \rightarrow 0} \frac{f(x+h) - a(h)f(x)}{s(h)}. \quad (1.18)$$

This constrains the forms of a and s . Nonstandard FD approximations can be used to improve the accuracy of FD algorithms, as we shall soon see.

A special case of the general NS-FD approximation that is used throughout much of this book is the central NS-FD approximation, given as

$$\begin{aligned} f'(x) &\cong \frac{d_x^c f(x)}{s(h)} \\ &= \frac{f(x+h/2) - f(x-h/2)}{s(h)}. \end{aligned} \quad (1.19)$$

1.2.1 Exact nonstandard finite difference expressions

With respect to certain sets of functions, it is possible to define exact NS-FD expressions for the derivative. For example, let $f(x) = e^{ikx}$ in Eq. (1.19). We find that $d_x^c e^{ikx} = 2i \sin(kh/2)$; thus, an exact central NS-FD expression for f' is

$$f'(x) = \frac{d_x^c f(x)}{s(h)}, \quad (1.20)$$

where

$$s(h) = \frac{2 \sin(kh/2)}{k}, \quad (1.21)$$

and k is any complex number. Equation (1.20) together with Eq. (1.21) is an exact FD expression even when h is not infinitesimal. As $h \rightarrow 0$, $s(h) \rightarrow h$;

hence, Eq. (1.20) together with Eq. (1.21) constitutes a permissible FD expression for the derivative with respect to exponential functions.

Any differential equation with solutions of the form $\psi(x) = a_+ e^{ikx} + a_- e^{-ikx}$ can be exactly modeled with central NS-FD expressions (and hence solved exactly with an FD algorithm).

Notice that in Eq. (1.21) s is independent of x . A NS-FD expression in which s depends on x is useless in a practical algorithm. For example, if $f(x) = x^n = e^{[n \ln(x)]}$, $n \neq 0$ and $x > 0$, an exact central NS-FD expression is

$$f'(x) = \frac{d_x^c f(x)}{s(x, h)}, \quad (1.22)$$

where

$$s(x, h) = \frac{2 \sinh[n \ln(x) h/2]}{n \ln(x)}. \quad (1.23)$$

Although Eq. (1.23) does converge to $f'(x)$ in the limit $h \rightarrow 0$, the dependence of s on x and the restriction $x > 0$ render this NS-FD expression useless to model differential equations with solutions of the form

$$\psi(x) = \sum_n a_n x^n. \quad (1.24)$$

1.2.2 Terminology

Henceforth, we refer to the FD expressions introduced in Section 1.1 as standard (S) FD expressions to distinguish them from the nonstandard (NS) expressions introduced in this section.

Often, for the sake of notational simplicity, we drop the superscript “c” for the central difference operators so that $d^c \rightarrow d$.

1.3 Standard Finite Difference Expressions for the Laplacian

We now omit the superscript “c” for the central difference operators, and $d_u = d_u^c$ for any variable u unless otherwise specified. The Laplacian operator $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$ has several different FD representations.

1.3.1 Two dimensions

In two dimensions, where $\nabla^2 = \partial_x^2 + \partial_y^2$, the most obvious FD approximation is

$$\nabla^2 f(\mathbf{x}) \cong \frac{\mathbf{d}^2}{h^2} f(\mathbf{x}), \quad (1.25)$$

where $\mathbf{d}^2 = d_x^2 + d_y^2$; d_x and d_y are partial central difference operators of the form in Eq. (1.8). Expanding $\mathbf{d}^2 f(x)$ gives

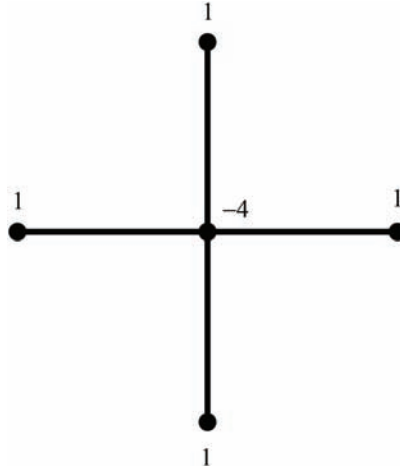


Figure 1.3 Computational molecule for $\mathbf{d}^2$.

$$\begin{aligned} \mathbf{d}^2 f(\mathbf{x}) = & f(x+h, y) + f(x-h, y) + f(x, y+h) \\ & + f(x, y-h) - 4f(x, y), \end{aligned} \quad (1.26)$$

and its computational molecule is depicted in Fig. 1.3; see Eq. (A1.1.17) for a deeper analysis of the significance of $\mathbf{d}^2$.

Using the points diagonally adjacent to (x, y) , we can construct another second-order S-FD approximation given by

$$\nabla^2 f(\mathbf{x}) \cong \frac{\mathbf{d}'^2}{h^2} f(\mathbf{x}), \quad (1.27)$$

where

$$\begin{aligned} 2\mathbf{d}'^2 f(\mathbf{x}) = & f(x+h, y+h) + f(x+h, y-h) \\ & + f(x-h, y+h) + f(x-h, y-h) - 4f(x, y). \end{aligned} \quad (1.28)$$

The factor of 2 in Eq. (1.28) takes into account the distance from (x, y) to $(x \pm h, y \pm h)$, which is $h\sqrt{2}$. The computational molecule of $\mathbf{d}'^2$ is shown in Fig. 1.4.

Now let $0 \leq g \leq 1$ be a parameter; then a family of second-order FD approximations to ∇^2 is

$$\nabla^2 \cong \frac{g\mathbf{d}^2 + (1-g)\mathbf{d}'^2}{h^2}. \quad (1.29)$$

The computational molecule for $\mathbf{d}_g^2 = g\mathbf{d}^2 + (1-g)\mathbf{d}'^2$ is shown in Fig. 1.5. From the definition Eq. (1.11), we have the identity

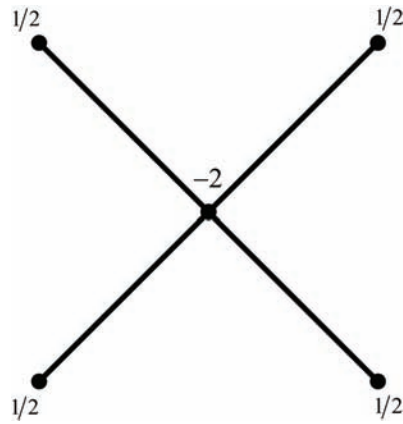


Figure 1.4 Computational molecule for $\mathbf{d}'^2$.

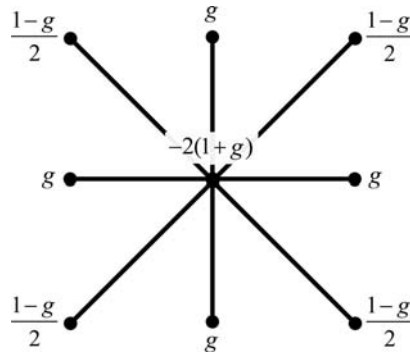


Figure 1.5 Computational molecule for $\mathbf{d}_g^2 = g\mathbf{d}^2 + (1-g)\mathbf{d}'^2$.

$$f(x+h) + f(x-h) = d_x^2 f(x) + 2f(x). \quad (1.30)$$

Applying Eq. (1.11) to $2\mathbf{d}'^2 f(\mathbf{x}) + 4f(\mathbf{x})$, we obtain

$$\begin{aligned} 2\mathbf{d}'^2 f(\mathbf{x}) + 4f(\mathbf{x}) &= f(x+h, y+h) + f(x-h, y+h) + f(x+h, y-h) \\ &\quad + f(x-h, y-h) \\ &= d_x^2 [f(x, y+h) + f(x, y-h)] + 2[f(x, y+h) + f(x, y-h)] \\ &= d_x^2 [d_y^2 f(x, y) + 2f(x, y)] + 2[d_y^2 f(x, y) + 2f(x, y)] \\ &= d_x^2 d_y^2 f(x, y) + 2[d_x^2 + d_y^2]f(x, y) + 4f(x, y). \end{aligned} \quad (1.31)$$

Thus,

$$\begin{aligned}\mathbf{d}'^2 &= d_x^2 + d_y^2 + \frac{1}{2}d_x^2 d_y^2 \\ &= \mathbf{d}^2 + \frac{1}{2}d_x^2 d_y^2.\end{aligned}\quad (1.32)$$

See Eq. (A1.1.15) for a further analysis of the significance of $\mathbf{d}'^2$. Hence, the most general S-FD operator for the Laplacian is

$$\mathbf{d}_\gamma^2 = \mathbf{d}^2 + \gamma d_x^2 d_y^2, \quad (1.33)$$

where γ is a parameter, and the most general S-FD approximation to ∇^2 is

$$\nabla^2 f(\mathbf{x}) \cong \frac{\mathbf{d}_\gamma^2}{h^2}. \quad (1.34)$$

The term $\mathbf{d}^2/h^2$ is a valid approximation of ∇^2 because $\lim_{h \rightarrow 0} [\mathbf{d}^2 f(\mathbf{x})/h^2] = \nabla^2 f(\mathbf{x})$. Since $d_x^2 d_y^2 f(\mathbf{x}) = h^4 \partial_x^2 \partial_y^2 f(\mathbf{x}) + \dots$, $\lim_{h \rightarrow 0} d_x^2 d_y^2 f(\mathbf{x})/h^2 = \lim_{h \rightarrow 0} [h^2 \partial_x^2 \partial_y^2 f(\mathbf{x})] = 0$; thus, $\lim_{h \rightarrow 0} [\mathbf{d}_\gamma^2 f(\mathbf{x})/h^2] = \nabla^2 f(\mathbf{x})$. This is true regardless of the value of γ , so γ is a free parameter.

As we shall later see, when h is not infinitesimal, the value of γ can be chosen such that the error of the finite difference expression is minimized with respect to certain classes of functions.

1.3.2 Three dimensions

In three dimensions, $\mathbf{d}^2 = d_x^2 + d_y^2 + d_z^2$ and

$$\begin{aligned}\mathbf{d}^2 f(\mathbf{x}) &= f(x+h, y, z) + f(x-h, y, z) + f(x, y+h, z) + f(x, y-h, z) \\ &\quad + f(x, y, z+h) + f(x, y, z-h) - 6f(x, y, z).\end{aligned}\quad (1.35)$$

Now there are two additional FD operators, $\mathbf{d}'^2$ and $\mathbf{d}''^2$, given by

$$\begin{aligned}4\mathbf{d}'^2 f(\mathbf{x}) &= f(x, y+h, z+h) + f(x, y-h, z+h) \\ &\quad + f(x, y+h, z-h) + f(x, y-h, z-h) \\ &\quad + f(x+h, y, z+h) + f(x-h, y, z+h) \\ &\quad + f(x+h, y, z-h) + f(x-h, y, z-h) \\ &\quad + f(x+h, y+h, z) + f(x-h, y+h, z) \\ &\quad + f(x+h, y-h, z) + f(x-h, y-h, z) - 12f(x, y, z),\end{aligned}\quad (1.36)$$

and

$$\begin{aligned}
 4\mathbf{d}''^2 f(\mathbf{x}) = & f(x+h, y+h, z+h) + f(x-h, y-h, z-h) \\
 & + f(x+h, y-h, z+h) + f(x-h, y+h, z-h) \\
 & + f(x-h, y+h, z+h) + f(x+h, y-h, z-h) \\
 & + f(x-h, y-h, z+h) + f(x+h, y+h, z-h) - 8f(x, y, z). \quad (1.37)
 \end{aligned}$$

Thus,

$$\nabla^2 \cong \frac{\mathbf{d}'^2}{h^2}, \quad (1.38)$$

$$\nabla^2 \cong \frac{\mathbf{d}''^2}{h^2}. \quad (1.39)$$

Again using identity Eq. (1.30), it can be shown that

$$\mathbf{d}'^2 = \mathbf{d}^2 + \frac{1}{4}(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2), \quad (1.40)$$

$$\mathbf{d}''^2 = \mathbf{d}^2 + \frac{1}{2}(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \frac{1}{4}d_x^2 d_y^2 d_z^2, \quad (1.41)$$

and the most general second-order FD operator for ∇^2 in three dimensions is

$$\mathbf{d}_\gamma^2 = \mathbf{d}^2 + \gamma_1(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \gamma_2 d_x^2 d_y^2 d_z^2, \quad (1.42)$$

where $\gamma = (\gamma_1, \gamma_2)$ is arbitrary. The most general S-FD expression is thus

$$\nabla^2 \cong \frac{\mathbf{d}_\gamma^2}{h^2}. \quad (1.43)$$

1.4 Nonstandard Finite Difference Expressions for the Laplacian

Since solutions of the wave equation and Maxwell's equations can be expressed in terms of Fourier components, it is of great interest to find FD expressions for ∇^2 that are accurate with respect to $e^{i\mathbf{k} \cdot \mathbf{x}}$, where $\mathbf{k} = (k_x, k_y, k_z)$.

In Section 1.2.1 it was shown that

$$d_x e^{ik_x} / e^{ik_x} = 2i \sin(kh/2) \Rightarrow d_x^2 e^{ik_x} / e^{ik_x} = -4 \sin^2(kh/2)$$

and thus $d_x^2 / s(h)^2 = \partial_x^2 e^{ik_x}$, exactly, where $s(h) = 2 \sin(kh/2) / k$.

Evaluating $\mathbf{d}^2 e^{i\mathbf{k}\cdot\mathbf{x}}$, we find that

$$\frac{\mathbf{d}^2 e^{i\mathbf{k}\cdot\mathbf{x}}}{e^{i\mathbf{k}\cdot\mathbf{x}}} = -4[\sin^2(k_x h/2) + \sin^2(k_y h/2) + \sin^2(k_z h/2)]; \quad (1.44)$$

thus,

$$\frac{\mathbf{d}^2 e^{i\mathbf{k}\cdot\mathbf{x}}}{s(h, \mathbf{k})^2} = \nabla^2 e^{i\mathbf{k}\cdot\mathbf{x}}, \quad (1.45)$$

exactly, where

$$s(h, \mathbf{k})^2 = \frac{4[\sin^2(k_x h/2) + \sin^2(k_y h/2) + \sin^2(k_z h/2)]}{k^2}, \quad (1.46)$$

and $k^2 = |\mathbf{k}|^2 = k_x^2 + k_y^2 + k_z^2$.

Although Eq. (1.45) is an exact NS-FD expression, it is unsatisfactory because it is exact only for one direction of $\mathbf{k}$. We would like an expression that is exact for all $\mathbf{k}$ directions. Unfortunately, this is impossible, but it is possible to find an NS-FD expression that is much more accurate than the S-FD expression of Eq. (1.25).

1.4.1 Two dimensions

Using the general S-FD operator $\mathbf{d}_\gamma^2$ given by Eq. (1.33), let us seek a value of γ such that $\mathbf{d}_\gamma^2 e^{i\mathbf{k}\cdot\mathbf{x}} = -4\sin^2(kh/2) e^{i\mathbf{k}\cdot\mathbf{x}}$, independently of the direction of $\mathbf{k}$. That is, we want

$$\begin{aligned} \frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\cdot\mathbf{x}}}{e^{i\mathbf{k}\cdot\mathbf{x}}} + 4\sin^2(kh/2) &= \frac{(d_x^2 + d_y^2 + \gamma d_x^2 d_y^2) e^{i\mathbf{k}\cdot\mathbf{x}}}{e^{i\mathbf{k}\cdot\mathbf{x}}} + 4\sin^2(kh/2) \\ &= 0 \end{aligned} \quad (1.47)$$

for some value of γ . Evaluating the right side of Eq. (1.47), we obtain

$$\begin{aligned} \frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k}\cdot\mathbf{x}}}{e^{i\mathbf{k}\cdot\mathbf{x}}} + 4\sin^2(kh/2) &= 4[\sin^2(kh/2) - \sin^2(k_x h/2) \\ &\quad - \sin^2(k_y h/2)] + 16\gamma \sin^2(k_x h/2) \sin^2(k_y h/2), \end{aligned} \quad (1.48)$$

where $(k_x, k_y) = k(\cos\theta, \sin\theta)$. The right side of Eq. (1.48) can be made to vanish with the choice $\gamma = \gamma(k_x, k_y)$, where

$$\gamma(k_x, k_y) = \frac{\sin^2(k_x h/2) + \sin^2(k_y h/2) - \sin^2(kh/2)}{4\sin^2(k_x h/2)\sin^2(k_y h/2)}. \quad (1.49)$$

Expanding Eq. (1.49) in a Taylor series about $kh = 0$, we find that

$$\gamma = \frac{1}{6} + \frac{(kh)^2}{180} + \frac{(kh)^4}{16} \left[\frac{19}{7560} + \frac{\cos(4\theta)}{1512} \right] + \dots \quad (1.50)$$

Although γ is not independent of the $\mathbf{k}$ direction, its dependence is weak, and thus for practical discretizations ($0 < kh < 1$), the fourth-order terms in kh , $O(kh)^4$, and higher orders, can be dropped, leaving

$$\gamma = \frac{1}{6} + \frac{(kh)^2}{180}. \quad (1.51)$$

Now inserting $\gamma = 1/6$ into Eq. (1.48) and expanding the right side in a Taylor series about $kh = 0$, we find that

$$\frac{\mathbf{d}_{1/6}^2 e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2) = \frac{(kh)^6}{1440} [1 - \cos(4\theta)] + \dots \quad (1.52)$$

Next, taking $\gamma = 1/6 + (kh)^2/180$ in Eq. (1.48), we find that

$$\begin{aligned} \frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2) = \\ - \frac{(kh)^8}{2^8} \left[\frac{127}{30240} - \frac{11}{2520} \cos(4\theta) + \frac{1}{6048} \cos(8\theta) \right] + \dots \end{aligned} \quad (1.53)$$

A simple calculation shows that the maximum deviation of $\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}} / e^{i\mathbf{k} \cdot \mathbf{x}}$ from $-4 \sin^2(kh/2)$ is

$$\max \left| \frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2) \right| = \frac{11}{322560} (kh)^8. \quad (1.54)$$

We have shown² that for $\gamma = \gamma'$, where $\gamma' = \gamma(k'_x, k'_y)$ and $(k'_x, k'_y) = k(2^{-1/4}, \sqrt{1 - 2^{-1/2}})$, the deviation from $4 \sin^2(kh/2)$ is even further reduced; however, in practical calculations, it is sufficient to take the value of γ given by Eq. (1.51), and often it is sufficient to use $\gamma = 1/6$.

For practical purposes, $\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}} / e^{i\mathbf{k} \cdot \mathbf{x}} = 4 \sin^2(kh/2)$ is an excellent approximation; thus, a nearly exact NS-FD approximation with respect to $e^{i\mathbf{k} \cdot \mathbf{x}}$ is

$$\nabla^2 \cong \frac{\mathbf{d}_\gamma^2}{s(h)^2}, \quad (1.55)$$

where $s(h) = 2 \sin(kh/2)/k$, as in the one-dimensional (1D) case. Defining the relative error of the NS-FD approximation for ∇^2 with respect to $e^{i\mathbf{k} \cdot \mathbf{x}}$ as

$$\begin{aligned}
\varepsilon_{\text{NS}}(\gamma) &= \frac{1}{\nabla^2 e^{i\mathbf{k} \cdot \mathbf{x}}} \left[\frac{\mathbf{d}_\gamma^2}{s(h)^2} - \nabla^2 \right] e^{i\mathbf{k} \cdot \mathbf{x}} \\
&= - \frac{\left[4 \sin^2(kh/2) + \mathbf{d}_\gamma^2 \right] e^{i\mathbf{k} \cdot \mathbf{x}}}{4 \sin^2(kh/2) e^{i\mathbf{k} \cdot \mathbf{x}}}, \tag{1.56}
\end{aligned}$$

and expanding ε_{NS} in a Taylor series about $kh = 0$, we find that

$$\varepsilon_{\text{NS}}(1/6) = \frac{(kh)^4}{1440} [1 - \cos(4\theta)] + \cdots, \tag{1.57}$$

$$\varepsilon_{\text{NS}}(1/6 + (kh)^2/180) = \frac{(kh)^6}{256} \left[\frac{11}{2520} - \frac{\cos(4\theta)}{270} - \frac{\cos(8\theta)}{1512} \right] + \cdots. \tag{1.58}$$

A simple calculation shows that the maximum error of the NS-FD Laplacian expression is

$$\max |\varepsilon_{\text{NS}}[1/6 + (kh)^2/180]| = \frac{1}{34560} (kh)^6. \tag{1.59}$$

On the other hand, the error of the S-FD expression is

$$\begin{aligned}
\varepsilon_{\text{S}} &= \frac{1}{\nabla^2 e^{i\mathbf{k} \cdot \mathbf{x}}} \left(\frac{\mathbf{d}^2}{h^2} - \nabla^2 \right) e^{i\mathbf{k} \cdot \mathbf{x}} \\
&= - \left[\frac{((kh)^2 + \mathbf{d}^2) e^{i\mathbf{k} \cdot \mathbf{x}}}{(kh)^2 e^{i\mathbf{k} \cdot \mathbf{x}}} \right] \\
&= - \frac{(kh)^2}{16} \left[1 + \frac{\cos(4\theta)}{3} \right] + \cdots. \tag{1.60}
\end{aligned}$$

In conclusion, by cleverly combining second-order FD operators, we can construct NS-FD expressions for $\nabla^2 e^{i\mathbf{k} \cdot \mathbf{x}}$ with up to sixth-order accuracy.

1.4.2 Three dimensions

The above developments in two dimensions can be extended to three. In spherical coordinates (θ and φ) $\mathbf{k} = k(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$. The deviation of $\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}} / e^{i\mathbf{k} \cdot \mathbf{x}}$ from $-4\sin^2(kh/2)$ is

$$\begin{aligned}
& \frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2) \\
&= \frac{\left[d_x^2 + d_y^2 + d_z^2 + \gamma_1 (d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \gamma_2 d_x^2 d_y^2 d_z^2 \right] e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2),
\end{aligned} \tag{1.61}$$

where $\gamma = (\gamma_1, \gamma_2)$. Expanding Eq. (1.61) in a Taylor series about $kh = 0$, we find that

$$\begin{aligned}
& \frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2) = -\frac{(kh)^4}{48} (6\gamma_1 - 1) \sin^2(\theta) \\
& \quad \times \left[\frac{\sin^2(2\varphi + \theta)}{2} + \frac{\sin^2(2\varphi - \theta)}{2} - \sin^2(2\varphi) + 7\sin^2(\theta) - 8 \right] \\
& \quad + O(kh)^6 + \dots.
\end{aligned} \tag{1.62}$$

Thus, setting $\gamma_1 = 1/6$ causes the $(kh)^4$ term to vanish, regardless of the value of γ_2 . Now taking $\gamma = [1/6 + \alpha(kh/2)^2, \gamma_2]$ in Eq. (1.62), we seek α and γ_2 such that the $(kh)^6$ term vanishes. Carrying out expansion in Eq. (1.62) to the sixth order in kh , we see that $-9\alpha + \gamma_2 + 1/6 = 0$, which implies that $\gamma_2 = 9\alpha - 1/6$ so that the constant (non-angular dependent) part of the $(kh)^6$ term vanishes. Setting $\gamma = (1/6 + \alpha(kh/2)^2, 9\alpha - 1/6)$ in Eq. (1.62), we find that

$$\begin{aligned}
& \frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2) = \left(\alpha - \frac{1}{45} \right) \frac{(kh)^6}{64} \\
& \quad \times [\sin^4\theta \sin^2(2\varphi)(1 - 36\cos^2\theta) + \sin^2(2\theta)] + \dots.
\end{aligned} \tag{1.63}$$

Thus, taking $\alpha = 1/45$ eliminates the $(kh)^6$ term, leaving only higher-order terms. Taking

$$\gamma_1 = \frac{1}{6} + \frac{(kh)^2}{180}, \tag{1.64a}$$

$$\gamma_2 = \frac{1}{30}, \tag{1.64b}$$

we obtain

$$\frac{\mathbf{d}_\gamma^2 e^{i\mathbf{k} \cdot \mathbf{x}}}{e^{i\mathbf{k} \cdot \mathbf{x}}} + 4 \sin^2(kh/2) = O(kh/2)^8. \tag{1.65}$$

We find that

$$\varepsilon_{\text{NS}}[1/6 + (kh)^2/180, 1/30] = (kh/2)^6 \times [\text{complicated expressions in } \theta \text{ and } \varphi]. \quad (1.66)$$

On the other hand, the S-FD error is

$$\varepsilon_{\text{S}} = (kh/2)^2 \times [\text{complicated expressions in } \theta \text{ and } \varphi]. \quad (1.67)$$

Thus motivated, we now define the NS Laplacian operator to be

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \left[\frac{1}{6} + \frac{(kh)^2}{180} \right] (d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \frac{1}{30} d_x^2 d_y^2 d_z^2. \quad (1.68)$$

In two dimensions, where $d_z^2 = 0$, this definition reduces to

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \left[\frac{1}{6} + \frac{(kh)^2}{180} \right] d_x^2 d_y^2. \quad (1.69)$$

As we have seen, $\tilde{\mathbf{d}}^2 e^{i\mathbf{k} \cdot \mathbf{x}} / e^{i\mathbf{k} \cdot \mathbf{x}} = 4 \sin^2(kh/2)$ almost exactly for any practical discretization when $0 < kh < 1$; hence,

$$\frac{\tilde{\mathbf{d}}^2}{s(h)^2} e^{i\mathbf{k} \cdot \mathbf{x}} = \nabla^2 e^{i\mathbf{k} \cdot \mathbf{x}}. \quad (1.70)$$

almost exactly, where $s(h) = 2\sin(kh/2)/k$, and the error is $O(kh)/2^8$.

Note 1.1

Consider a medium in which the refractive index is piecewise constant, ranging from $n = 1$ (the ambient medium) to n_s (in a “scatterer”). The local wavenumber thus lies between k_0 and $n_s k_0$. In many practical FDTD calculations, it is sufficient to take

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \left[\frac{1}{6} + \frac{(k_0 h)^2}{180} \right] (d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \frac{1}{30} d_x^2 d_y^2 d_z^2, \quad (1.71)$$

so that $\tilde{\mathbf{d}}^2$ is not a function of position. In fact, for sufficiently small $k_0 h$, we can simply take

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \frac{1}{6} (d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \frac{1}{30} d_x^2 d_y^2 d_z^2. \quad (1.72)$$

The last term of Eq. (1.72), although small, is needed to ensure the stability of NS-FDTD.

1.5 Factoring the Nonstandard Finite Difference Laplacian

To construct an NS-FD algorithm to solve Maxwell's equations, we would like to find a NS-difference operator $\mathbf{d}'$, such that $\mathbf{d}' \bullet \mathbf{d}' = \tilde{\mathbf{d}}^2$. Unfortunately, this is impossible. Although $\mathbf{d} \bullet \mathbf{d} = \mathbf{d}^2$, $\mathbf{d}'$ does not exist, but we can find $\tilde{\mathbf{d}}$ such that $\mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d} = \tilde{\mathbf{d}}^2$ (but $\tilde{\mathbf{d}} \bullet \tilde{\mathbf{d}} \neq \tilde{\mathbf{d}}^2$).

1.5.1 Two dimensions

As we have seen, for function $f(x, y)$, $\partial_x f \cong d_x f/h$. There is another FD approximation given by $\partial_x f \cong d'_x f/h$, where

$$2d'_x f(x, y) = f(x + h/2, y + h) + f(x + h/2, y - h) - [f(x - h/2, y + h) + f(x - h/2, y - h)]. \quad (1.73)$$

Similarly, $\partial_y f \cong d'_y f/h$, where

$$2d'_y f(x, y) = f(x + h, y + h/2) + f(x - h, y + h/2) - [f(x + h, y - h/2) + f(x - h, y - h/2)]. \quad (1.74)$$

Using identity Eq. (1.30), it is easy to show that

$$d'_x = d_x \left(1 + \frac{1}{2} d_y^2 \right), \quad (1.75a)$$

$$d'_y = d_y \left(1 + \frac{1}{2} d_x^2 \right). \quad (1.75b)$$

Forming the vector difference operator $\mathbf{d}' = (d'_x, d'_y)$ and defining $\tilde{\mathbf{d}} = (\tilde{d}_x, \tilde{d}_y)$, we postulate the form $\tilde{\mathbf{d}} = \mathbf{d} + \alpha(d_x d_y^2, d_y d_x^2)$, or

$$\tilde{d}_x = d_x + \alpha d_y^2, \quad (1.76a)$$

$$\tilde{d}_y = d_y + \alpha d_x^2. \quad (1.76b)$$

Requiring that $\mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d} = \tilde{\mathbf{d}}^2$, we find that

$$\alpha = \frac{1}{12} + \frac{(kh)^2}{360}. \quad (1.77)$$

1.5.2 Three dimensions

In three dimensions, besides $\partial_x f \cong d_x f/h$, there are two additional FD expressions, $\partial_x f \cong d'_x f/h$ and $\partial_x f \cong d''_x f/h$, where

$$\begin{aligned}
4d'_x f(x, y, z) = & f(x + h/2, y + h, z + h) + f(x + h/2, y + h, z - h) \\
& + f(x + h/2, y - h, z + h) + f(x + h/2, y - h, z - h) \\
& - f(x - h/2, y + h, z + h) - f(x - h/2, y + h, z - h) \\
& - f(x - h/2, y - h, z + h) - f(x - h/2, y - h, z - h), \quad (1.78)
\end{aligned}$$

$$\begin{aligned}
4d''_x f(x, y, z) = & f(x + h/2, y + h, z) + f(x + h/2, y - h, z) \\
& + f(x + h/2, y, z + h) + f(x + h/2, y, z - h) \\
& - f(x - h/2, y + h, z) - f(x - h/2, y - h, z) \\
& - f(x - h/2, y, z + h) - f(x - h/2, y, z - h). \quad (1.79)
\end{aligned}$$

The corresponding difference operators for ∂_y and ∂_z can be found by analogy with ∂_x . Using Eq. (1.30), it can be straightforwardly shown that

$$d'_x = d_x \left(1 + \frac{d_y^2 + d_z^2}{2} + \frac{d_y^2 d_z^2}{4} \right), \quad (1.80a)$$

$$d'_y = d_y \left(1 + \frac{d_x^2 + d_z^2}{2} + \frac{d_x^2 d_z^2}{4} \right), \quad (1.80b)$$

$$d'_z = d_z \left(1 + \frac{d_x^2 + d_y^2}{2} + \frac{d_x^2 d_y^2}{4} \right), \quad (1.80c)$$

and

$$d''_x = d_x \left(1 + \frac{d_y^2 + d_z^2}{4} \right), \quad (1.81a)$$

$$d''_y = d_y \left(1 + \frac{d_x^2 + d_z^2}{4} \right), \quad (1.81b)$$

$$d''_z = d_z \left(1 + \frac{d_x^2 + d_y^2}{4} \right). \quad (1.81c)$$

Since we want the 3D form of $\tilde{\mathbf{d}}$ to reduce the 2D form for $d_z = 0$, we postulate that

$$\tilde{d}_x = d_x \left[1 + \alpha(d_y^2 + d_z^2) + \beta d_y^2 d_z^2 \right], \quad (1.82a)$$

$$\tilde{d}_y = d_y \left[1 + \alpha(d_x^2 + d_z^2) + \beta d_x^2 d_z^2 \right], \quad (1.82b)$$

$$\tilde{d}_z = d_z \left[1 + \alpha(d_x^2 + d_y^2) + \beta d_y^2 d_z^2 \right], \quad (1.82c)$$

where α is given by Eq. (1.77). Again requiring that $\mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d} = \tilde{\mathbf{d}}^2$, we find that $\beta = 1/90$. Thus,

$$\tilde{\mathbf{d}} = \mathbf{d} + \left(\frac{1}{12} + \frac{(kh)^2}{360} \right) \begin{bmatrix} d_x(d_y^2 + d_z^2) \\ d_y(d_x^2 + d_z^2) \\ d_z(d_x^2 + d_y^2) \end{bmatrix} + \frac{1}{90} \begin{bmatrix} d_x(d_y^2 d_z^2) \\ d_y(d_x^2 d_z^2) \\ d_z(d_x^2 d_y^2) \end{bmatrix}, \quad (1.83)$$

where the column matrices represent vector difference operators. The 2D form of $\tilde{\mathbf{d}}$ is obtained by setting $d_z = 0$ in Eq. (1.83).

This formulation will be used in Chapter 10.

Important Points of Chapter 1

- We introduce the notation to be used throughout this book:
Central partial difference operator:

$$d_x f(x, y) = f(x + h/2, y) - f(x - h/2, y).$$

Second partial difference operator:

$$d_x d_x = d_x^2, \quad d_x^2 f(x, y) = f(x + h, y) + f(x - h, y) - 2f(x, y).$$

Gradient difference operator:

$$\text{standard: } \mathbf{d} = (d_x, d_y, d_z); \text{ nonstandard: } \tilde{\mathbf{d}} = (\tilde{d}_x, \tilde{d}_y, \tilde{d}_z).$$

Laplacian difference operator:

$$\text{standard: } \mathbf{d}^2 = d_x^2 + d_y^2 + d_z^2; \text{ nonstandard: } \tilde{\mathbf{d}}^2 = \mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d}.$$

- Useful expressions:

$$\begin{aligned} d_x e^{ikx} &= 2i \sin(k\Delta x/2) \frac{k^2}{4 \sin^2(kh/2)} \tilde{\mathbf{d}}^2 e^{ik \bullet \mathbf{x}} \\ &= \nabla^2 e^{ik \bullet \mathbf{x}}, \text{ almost exactly.} \end{aligned}$$

- There exist exact finite difference expressions for the derivatives of the single-variable exponential functions.
- All finite difference expressions are equal (as $h \rightarrow 0$), but some finite difference expressions are more equal than others (for non-infinitesimal h).

Appendix 1.1 Mathematical Properties of Finite Difference Operators

We can gain useful insights by more closely examining the relationship between derivatives and finite difference expressions; this relationship also yields some useful expressions.

A1.1.1 Forward finite difference operator

Letting n be a positive integer, we express the definition of the derivative in the form

$$\frac{d}{dx}f(x) = \lim_{n \rightarrow \infty} \frac{f(x + h/n) - f(x)}{h/n}. \quad (\text{A1.1.1})$$

For large n ,

$$f(x + h/n) \cong \left(1 + \frac{h}{n} \partial_x\right) f(x), \quad (\text{A1.1.2})$$

where $\partial_x = d/dx$.

Readers who are familiar with Lie group theory will recognize ∂_x to be the generator of translations. Iterating Eq. (A1.1.2), we find that

$$\begin{aligned} f(x + 2h/n) &\cong \left(1 + \frac{h}{n} \partial_x\right) f(x + h/n) \\ &= \left(1 + \frac{h}{n} \partial_x\right)^2 f(x). \end{aligned} \quad (\text{A1.1.3})$$

By induction, we obtain

$$f(x + h) \cong \left(1 + \frac{h}{n} \partial_x\right)^n f(x), \quad (\text{A1.1.4})$$

and in the limit $n \rightarrow \infty$,

$$f(x + h) = e^{h\partial_x} f(x). \quad (\text{A1.1.5})$$

Equation (A1.1.5) is the Taylor series expansion of $f(x + h)$ about x , and $e^{h\partial_x}$ is the Lie group element that produces the translation $x \rightarrow x + h$.

Thus, the forward difference $d_x^f f(x) = f(x + h) - f(x)$ is given by

$$d_x^f f(x) = (e^{h\partial_x} - 1)f(x); \quad (\text{A1.1.6})$$

hence,

$$\begin{aligned} d_x^f &= e^{h\partial_x} - 1 \\ &= h\partial_x + \frac{1}{2!}h^2\partial_x^2 + \frac{1}{3!}h^3\partial_x^3 + \cdots. \end{aligned} \quad (\text{A1.1.7})$$

Solving for ∂_x in terms of FD operators, we obtain

$$\begin{aligned}\partial_x &= \frac{\ln(1 + d_x^f)}{h} \\ &= \frac{1}{h} \left[d_x^f - \frac{(d_x^f)^2}{2} + \frac{(d_x^f)^3}{3} \mp \cdots \right].\end{aligned}\quad (\text{A1.1.8})$$

Thus, the differential equation $\partial_x f(x) = g(x)$ is equivalent to the difference equation $[d_x^f - (d_x^f)^2/2 \pm \cdots]f(x) = hg(x)$; likewise, the difference equation $d_x^f f(x) = hg(x)$ is equivalent to the differential equation $[\partial_x + h\partial_x^2/2 + \cdots]f(x) = g(x)$. It is therefore not surprising that the solution of a differential equation generally differs from that of its difference equation model.

A1.1.2 Central finite difference operator

We can derive similar expressions for the central FD operators. Using the results above, we find that

$$\begin{aligned}d_x^c &= [e^{(h/2)\partial_x} - e^{-(h/2)\partial_x}]f(x) \\ &= 2 \sinh[(h/2)\partial_x]f(x).\end{aligned}\quad (\text{A1.1.9})$$

Hence, the central FD operator can be expressed in terms of derivatives as

$$\begin{aligned}d_x^c &= 2 \sinh[(h/2)\partial_x] \\ &= h\partial_x + \frac{1}{24}h^3\partial_x^3 + \frac{1}{1920}h^5\partial_x^5.\end{aligned}\quad (\text{A1.1.10})$$

It is easily seen from the above that

$$\begin{aligned}(d_x^c)^2 &= 4 \sinh^2[(h/2)\partial_x] \\ &= h^2\partial_x^2 + \frac{1}{12}h^4\partial_x^4 + \frac{1}{360}h^6\partial_x^6 + \cdots.\end{aligned}\quad (\text{A1.1.11})$$

Solving Eq. (A1.1.11) for ∂_x , the expansion of the derivative in terms of central FD operators is

$$\begin{aligned}\partial_x &= \frac{1}{h} 2 \sinh^{-1}(d_x^c/2) \\ &= \frac{1}{h} \left[d_x^c - \frac{1}{24}(d_x^c)^3 + \frac{3}{640}(d_x^c)^5 \mp \cdots \right].\end{aligned}\quad (\text{A1.1.12})$$

From Eq. (A1.1.12), we find that

$$\begin{aligned}\partial_x^2 &= \frac{1}{h^2} 4[\sinh^{-1}(d_x^c/2)]^2 \\ &= \frac{1}{h^2} \left[(d_x^c)^2 - \frac{1}{12} (d_x^c)^4 + \frac{1}{90} (d_x^c)^6 \mp \cdots \right].\end{aligned}\quad (\text{A1.1.13})$$

A1.1.3 Multiple variables

Equation (A1.1.5) can be generalized to the case of several variables:

$$f(x + h_x, y + h_y + z + h_z) = e^{h_x \partial_x + h_y \partial_y + h_z \partial_z} f(x, y, x). \quad (\text{A1.1.14})$$

For example, $2\mathbf{d}'^2 f(x)$ in Eq. (1.28),

$$\begin{aligned}2\mathbf{d}'^2 f(\mathbf{x}) &= f(x + h, y + h) + f(x + h, y - h) \\ &\quad + f(x - h, y + h) + f(x - h, y - h) - 4f(x, y),\end{aligned}$$

is equivalent to

$$\begin{aligned}2\mathbf{d}'^2 f(\mathbf{x}) &= [e^{h\partial_x + h\partial_y} + e^{-(h\partial_x + h\partial_y)} + e^{h\partial_x - h\partial_y} + e^{-(h\partial_x - h\partial_y)} - 4]f(x, y) \\ &= 2[\cosh(h\partial_x + h\partial_y) + \cosh(h\partial_x - h\partial_y) - 2]f(x, y) \\ &= \left\{ h^2 (\partial_x^2 + \partial_y^2) + h^4 \left[\frac{1}{12} (\partial_x^4 + \partial_y^4) + \frac{1}{2} \partial_x^2 \partial_y^2 \right] + \cdots \right\} f(x, y).\end{aligned}\quad (\text{A1.1.15})$$

On the other hand,

$$\begin{aligned}\mathbf{d}^2 f(\mathbf{x}) &= f(x + h, y) + f(x - h, y) + f(x, y + h) \\ &\quad + f(x, y - h) - 4f(x, y)\end{aligned}\quad (\text{A1.1.16})$$

is equivalent to

$$\begin{aligned}\mathbf{d}^2 f(\mathbf{x}) &= [e^{h\partial_x} + e^{-h\partial_x} + e^{h\partial_y} + e^{-h\partial_y} - 4]f(x, y) \\ &= 2[\cosh(h\partial_x) + \cosh(h\partial_y) - 2]f(x, y) \\ &= \left\{ h^2 (\partial_x^2 + \partial_y^2) + \frac{1}{12} h^4 (\partial_x^4 + \partial_y^4) + \cdots \right\} f(x, y).\end{aligned}\quad (\text{A1.1.17})$$

Appendix 1.2 Noninteger-Order Sums and Differences

Except for Note A1.2.1, this Appendix 1.2 is not directly relevant to the main text. We include it as a reference for those interested in modeling phenomena

outside the scope of this book. Certain physical phenomena (such as quantum entanglement) appear to be nonlocal, and it is interesting to note that noninteger-order differences and sums are also nonlocal.

Sums and differences can be extended to noninteger-order and are useful in modeling stochastic processes such as Brownian motion. Interesting insight can be gained by examining these generalizations.

Note that in this appendix, d denotes the forward finite difference.

A1.2.1 Noninteger-order summation

Let $x = \chi h$ and $f_\chi = f(\chi h)$, and define the summation operator by

$$Sf|_0^\chi = \sum_{i=0}^{\chi-1} f_i \quad (\text{A1.2.1})$$

in the limit

$$\lim_{h \rightarrow 0} h Sf|_0^\chi = \int_0^x dt f(t), \quad (\text{A1.2.2})$$

defining the double summation

$$S^2 f|_0^\chi = \sum_{i=0}^{\chi-1} \sum_{j=0}^i f_j, \quad (\text{A1.2.3})$$

where $\chi \geq 2$. Notice that in the second sum, j runs from 0 to i , not to $i - 1$. In the limit

$$\lim_{h \rightarrow 0} h^2 S^2 f|_0^\chi = \int_0^x dt \int_0^t dt' f(t'), \quad (\text{A1.2.4})$$

by definition,

$$\begin{aligned} \sum_{j=0}^0 f_j &= f_0, \\ \sum_{j=0}^1 f_j &= f_0 + f_1, \\ \sum_{j=0}^2 f_j &= f_0 + f_1 + f_2; \\ &\vdots \end{aligned} \quad (\text{A1.2.5})$$

thus,

$$\sum_{i=0}^{\chi-1} \sum_{j=0}^i f_j = \chi f_0 + (\chi - 1)f_1 + (\chi - 2)f_2 + \cdots + f_{\chi-1}, \quad (\text{A1.2.6})$$

and hence,

$$S^2 f|_0^\chi = \sum_{i=0}^{\chi-1} (\chi - i) f_i. \quad (\text{A1.2.7})$$

Notice the similarity of Eq. (A1.2.7) to the two-fold integral $I^2 f|_0^\chi = \int_0^\chi dt (x - t) f(t)$ given by Eq. (A2.2.3).

Evaluating the triple summation

$$S^3 f|_0^\chi = \sum_{i=0}^{\chi-1} \sum_{j=0}^i \sum_{k=0}^j f_k, \quad (\text{A1.2.8})$$

we find that

$$\begin{aligned} \sum_{j=0}^i \sum_{k=0}^j f_k &= f_0 \\ &\quad + f_0 + f_1 \\ &\quad + f_0 + f_1 + f_2 \\ &\quad + \\ &\quad \vdots \\ &\quad + f_0 + f_1 + \cdots + f_i \\ &= (i+1)f_0 + if_1 + (i-1)f_2 + \cdots + f_i \\ &= \sum_{j=0}^i (i+1-j)f_j. \end{aligned} \quad (\text{A1.2.9})$$

Thus,

$$\begin{aligned} \sum_{i=0}^{\chi-1} \sum_{j=0}^i \sum_{k=0}^j f_k &= f_0 \\ &\quad + 2f_0 + f_1 \\ &\quad + 3f_0 + 2f_1 + f_2 \\ &\quad \vdots \\ &\quad + \chi f_0 + (\chi-1)f_1 + (\chi-2)f_2 + \cdots + f_{\chi-1} \\ &= f_0 \frac{(\chi+1)\chi}{2} + f_1 \frac{\chi(\chi-1)}{2} + f_2 \frac{(\chi-1)(\chi-2)}{2} + \cdots + f_{\chi-1} \\ &= \frac{1}{2} \sum_{i=0}^{\chi-1} (\chi+1-i)(\chi-i)f_i. \end{aligned} \quad (\text{A1.2.10})$$

Therefore,

$$S^3 f|_0^\chi = \frac{1}{2} \sum_{i=0}^{\chi-1} \frac{(\chi+1-i)!}{(\chi-1-i)!} f_i. \quad (\text{A1.2.11})$$

By induction, we obtain

$$S^n f|_0^\chi = \frac{1}{(n-1)!} \sum_{i=0}^{\chi-1} \frac{(\chi+n-2-i)!}{(\chi-i-1)!} f_i. \quad (\text{A1.2.12})$$

Substituting Γ functions in place of the factorial functions, and using $\Gamma(n) = (n-1)!$, noninteger-order summation for $n \geq 0$ is defined by

$$S^n f|_0^\chi = \frac{1}{\Gamma(n)} \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi+n-1-i)}{\Gamma(\chi-i)} f_i. \quad (\text{A1.2.13})$$

Note A1.2.1

The Γ function³ is defined by

$$\Gamma(x) = \int_0^\infty dt e^{-t} t^{x-1}. \quad (\text{A1.2.14})$$

This definition is valid for noninteger arguments. When $n > 1$ is an integer, $\Gamma(n) = (n-1)!$. The Taylor expansion of $1/\Gamma(x)$ about $n = 0$ is

$$\frac{1}{\Gamma(x)} = x + \cdots; \quad (\text{A1.2.15})$$

hence,

$$\lim_{x \rightarrow 0} \frac{1}{\Gamma(x)} = 0. \quad (\text{A1.2.16})$$

From Eq. (A1.2.13), we have

$$S^0 f|_0^\chi = \frac{1}{\Gamma(0)} \left[\frac{\Gamma(N-1)}{\Gamma(N)} f_0 + \frac{\Gamma(N-2)}{\Gamma(N-1)} f_1 + \frac{\Gamma(N-3)}{\Gamma(N-2)} f_2 + \cdots \frac{\Gamma(0)}{\Gamma(1)} \right], \quad (\text{A1.2.17})$$

and using Eq. (A1.2.16), we find that

$$S^0 f|_0^\chi = f_{\chi-1}. \quad (\text{A1.2.18})$$

One might have hoped that $S^0 f|_0^\chi$ would be f_χ so that S^0 would be the identity operator **1**. However, $\lim_{h \rightarrow 0} f(\chi h - h) = f(\chi h) \Rightarrow \lim_{h \rightarrow 0} f_{\chi-1} = f_\chi$; thus, $\lim_{h \rightarrow 0} S^0 f|_0^\chi = f_\chi$ and, hence,

$$\lim_{h \rightarrow 0} S^0 = \mathbf{1}. \quad (\text{A1.2.19})$$

If the upper limit of the summation in Eq. (A1.2.1) were to taken to be χ instead of $\chi - 1$, we would have $S^0 f|_0^\chi = f_\chi$, but this would give (see Section A1.2.2) $dS^0 f|_0^\chi = f_{\chi+1}$ instead of f_χ (where $df_\chi = f_{\chi+1} - f_\chi$); thus, d would not be the inverse of S .

Example 1

Letting $f(x) = x$, $Sf|_0^\chi = h \sum_{i=0}^{\chi-1} i$ is the summation of an arithmetic series. $S^{1/2} f|_0^\chi$ is given by

$$\begin{aligned} S^{1/2} f|_0^\chi &= \frac{h}{\Gamma(1/2)} \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi - i - 1/2)}{\Gamma(\chi - i)} i \\ &= h \sum_{i=0}^{\chi-1} \frac{i}{(\chi - i - 1)!} \frac{1}{2^{\chi-i-1}} \prod_{j=0}^{\chi-i} |2j - 1|, \end{aligned} \quad (\text{A1.2.20})$$

where

$$\frac{\Gamma(n - 1/2)}{\Gamma(1/2)} = \frac{1}{2^{n-1}} \prod_{m=0}^{n-1} |2m - 1|. \quad (\text{A1.2.21})$$

Taking $\chi = 5$ and $h = 1$, we obtain the weighted sum,

$$\begin{aligned} S^{1/2} f|_0^5 &= \frac{3 \cdot 5 \cdot 7}{2^3 3!} \cdot 1 + \frac{3 \cdot 5}{2^2 2!} \cdot 2 + \frac{3}{2^1 1!} \cdot 3 + 4, \\ &= \frac{35}{16} \cdot 1 + \frac{15}{8} \cdot 2 + \frac{3}{2} \cdot 3 + 1 \cdot 4. \end{aligned} \quad (\text{A1.2.22})$$

Example 2

Taking $f(x) = \sin(\pi x/2.1)/e^{x/6} \sqrt{x+1} - (1 - e^{-x/30})\sqrt{x}$, $\chi = 10$, and $h = 1$, we plot $S^n f|_0^{10}$ versus n in Fig. A1.2.1. Here, n is real (not necessarily an integer); obviously, the noninteger sum is a smooth generalization from integer-order summation to noninteger-order summation.

A1.2.2 Noninteger-order differences

The forward finite difference operator d acting on f is defined by

$$df_\chi = f_{\chi+1} - f_\chi. \quad (\text{A1.2.23})$$

Iterating Eq. (A1.2.23) n fold, it is easy to show that

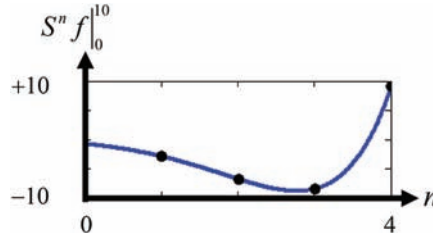


Figure A1.2.1 The integer and noninteger-order sums of Example 1.2. Dots denote integer-order sums, and lines denote noninteger-order sums.

$$d^n f_\chi = \sum_{\ell=0}^n \frac{(-1)^\ell n!}{(n-\ell)!\ell!} f_{\chi+n-\ell}, \quad (\text{A1.2.24})$$

where $n \geq 0$ is an integer.

Note A1.2.2

The substitution $f(x) \rightarrow f(x - nh/2) \Rightarrow f_{\chi+n-\ell} \rightarrow f_{\chi+(n/2)-\ell}$ in Eq. (A1.2.24) yields the n^{th} central difference. $d^c f_\chi = f_{\chi+1/2} - f_{\chi-1/2}$, and

$$(d^c)^2 f_\chi = f_{\chi+1} - 2f_\chi + f_{\chi-1}, \quad (\text{A1.2.25a})$$

$$(d^c)^3 f_\chi = f_{\chi+3/2} - 3f_{\chi+1/2} + 3f_{\chi-1/2} - f_{\chi-3/2}, \quad (\text{A1.2.25b})$$

$$(d^c)^4 f_\chi = f_{\chi+2} - 4f_{\chi+1} + 6f_\chi - 4f_{\chi-1} + f_{\chi-2}, \quad (\text{A1.2.25c})$$

etc.

Evaluating Eq. (A1.2.24) for $n = 0$ gives $d^0 f_\chi = f_\chi$; hence,

$$d^0 = \mathbf{1}. \quad (\text{A1.2.26})$$

It is easy to show that $dSf|_0^\chi = f_\chi \Rightarrow dS = \mathbf{1}$. Thus, d is the left inverse of S :

$$d = S_{\text{left}}^{-1}. \quad (\text{A1.2.27})$$

However, $Sd \neq dS$, thus, $Sd \neq \mathbf{1}$; instead,

$$\begin{aligned} Sd f|_0^\chi &= \sum_{\tau=0}^{\chi-1} [f_{\tau+1} - f_\tau] \\ &= f_\chi - f_0. \end{aligned} \quad (\text{A1.2.28})$$

Note A1.2.3

If the upper limit of the summation in Eq. (A1.2.1) had been taken to be χ instead of $\chi - 1$, then we would have had $dSf|_0^\chi = f_{\chi+1}$, and d would not be the left inverse of S .

We now proceed to extend the difference operation defined in Eq. (A1.2.24) to noninteger values. Simply replacing the factorial terms with Γ functions does not yield a useful definition. Instead, we make use of noninteger-order summation. Taking $0 \leq \nu < 1$, we define

$$d^\nu = dd^{\nu-1} = dd^{-(1-\nu)} = dS^{1-\nu}, \quad (\text{A1.2.29})$$

where $d^{-(1-\nu)} = S^{1-\nu}$ because d is the left inverse of S . Thus, from Eq. (A1.2.13),

$$\begin{aligned} d^\nu f_\chi &= \frac{1}{\Gamma(1-\nu)} d \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi-\nu-i)}{\Gamma(\chi-i)} f_i \\ &= f_\chi - \frac{\nu}{\Gamma(1-\nu)} \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi-\nu-i)}{\Gamma(\chi+1-i)} f_i. \end{aligned} \quad (\text{A1.2.30})$$

Setting $\nu = 0$ in Eq. (A1.2.30), we find that $d^0 f_\chi = f_\chi \Rightarrow d^0 = \mathbf{1}$, in accordance with Eq. (A1.2.26).

Next, using Eq. (A1.2.29), let us evaluate $d^1 f_\chi = \lim_{\nu \rightarrow 1} dS^{1-\nu} f|_0^\chi$, using $S^0 f|_0^\chi = f_{\chi-1} = f_{\chi-1}$ from Eq. (A1.2.18). This yields

$$df_\chi = f_\chi - f_{\chi-1}, \quad (\text{A1.2.31})$$

which contradicts the definition in Eq. (A1.2.23). The definition of a noninteger (ν^{th})-order difference [Eq. (A1.2.28)] is thus inconsistent with the definition of the integer-order difference in the limit $\nu = n \rightarrow 1$. However, since

$$\lim_{h \rightarrow 0} \frac{f_\chi - f_{\chi-1}}{h} = \lim_{h \rightarrow 0} \frac{f_{\chi+1} - f_\chi}{h} = f'(\chi), \quad (\text{A1.2.32})$$

d^ν , as defined by Eq. (A1.2.29), does converge to d in the double limits $h \rightarrow 0$ and $\nu \rightarrow 1$; that is,

$$\lim_{h \rightarrow 0} (\lim_{\nu \rightarrow 1} d^\nu) = d. \quad (\text{A1.2.33})$$

One could try to redefine the sum and difference operators to make $\lim_{\nu \rightarrow 1} d^\nu = d$ even when h is not infinitesimal, but this approach leads to much more complicated expressions that are not intuitively obvious.

For noninteger $n + \nu$, where $n \geq 0$ is an integer and $0 < \nu < 1$ is real, we define $d^{n+\nu}$ in two steps by

$$g_\chi = d^n f_\chi, \quad (\text{A1.2.34a})$$

$$d^{n+\nu} f_\chi = d^\nu g_\chi, \quad (\text{A1.2.34b})$$

where $d^n f_\chi$ is computed using Eq. (A1.2.24), and $d^\nu g_\chi$ is computed using Eq. (A1.2.30).

While for integer n , $d^n f_\chi$ depends only on the values of $f_{\chi+1}$ in the range $0 \leq i \leq n$, $d^{n+\nu} f_\chi$ depends on all the values of f_i in the range $0 \leq i \leq \chi + n$.

Example 3

Let $\chi = 5$, $h = 1$, and $f(x) = x^2$; then, $df_\chi = 2\chi h + h^2$. Using Eqs. (A1.2.29) and (A1.2.30) together with Eq. (A1.2.21), we find that

$$\begin{aligned} d^{1/2} f_\chi &= \chi^2 - \frac{1}{2\Gamma(1/2)} \sum_{i=0}^{\chi-1} \frac{\Gamma(\chi - i - 1/2)}{(\chi - i)!} i^2 \\ &= \chi^2 - \sum_{i=0}^{\chi-1} \frac{1}{(\chi - i)!} \frac{i^2}{2^{\chi-i}} \prod_{j=0}^{\chi-i} |2j - 1| \end{aligned} \quad (\text{A1.2.35})$$

Example 4

Let $f(x) = 10e^{-x/16} \sin(\pi x/8)$ and $1 \leq \chi \leq 32$, and plot $d^n f_\chi$ versus χ for different values of n . Figure A1.2.2 shows that as $0 < \varepsilon \rightarrow 0$, $\lim_{\varepsilon \rightarrow 0} d^{n+\varepsilon} f_\chi = d^n f_\chi$, but $\lim_{\varepsilon \rightarrow 0} d^{n-\varepsilon} f_\chi \neq d^2 f_\chi$. For example, $d^{2.01} f_\chi \cong d^2 f_\chi$, but $d^{1.99} f_\chi \not\cong d^2 f_\chi$.

Further details on noninteger sums and differences can be found in Ref. 4.

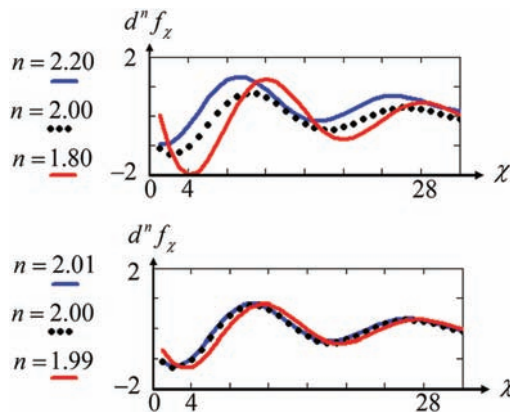


Figure A1.2.2 Integer and noninteger-order differences.

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Chapter 2

Accuracy, Stability, and Convergence of Numerical Algorithms

“Algorithm” is a late 17th century variant (influenced by the Greek *arithmos*, “number”) of the Middle English *algorism*, via Old French from medieval Latin *algorismus*. The latter comes from the Arabic, *al-Kwārizmī* ‘the man of *Kwārizm*’ (now Khiva), which was a name given to the 9th-century Persian mathematician Abū Ja‘far Muhammad ibn Mūsa, who wrote a book titled *On the Calculation with Hindu Numerals* in about 825 AD. This book was principally responsible for spreading the Indian system of numeration throughout the Middle East and Europe. It was translated into Latin as *Algoritmi de numero Indorum* (Al-Khwarizmi on the Hindu Art of Reckoning). *Algoritmi* in the book title became “algorithm.”¹

Many real phenomena are too complicated to comprehend, but we can attempt to understand them by constructing models that contain their essential features while ignoring minor complications. (What is essential is not always obvious, and the choice may depend on one’s purpose.) Models can yield deep insight into the nature of reality. A good model not only explains a phenomenon, but also predicts things yet to be observed. The quark model was devised in the early 1960s to simply explain the puzzling multiplicity of hadrons (that were being discovered) in terms of a few simple (presumed to be imaginary) elementary particles called quarks. No one believed that quarks actually existed, but later it was found that they do exist. It is remarkable indeed that the best model seems to be the simplest one that accounts for the facts—the principle of Occam’s razor.² The FDTD methodology, the main subject of this book, is appealing because of its simplicity.

Methodologies such as Feynman diagrams can take on lives of their own and even indicate new phenomena. A finite difference model of the logistic

equation, which gives the wrong solution, has been used to study chaos (see Section 2.6.1). It has even been proposed that reality itself is just a set of algorithms.³ Indeed, in this book we will encounter algorithms meant to solve one problem that lead to solutions and models of other problems that explain—at least heuristically—certain real physical phenomena.

Before embarking on the main topic of this book, we introduce a few example algorithms and analyze their accuracy and numerical stability. Our purpose is not only to show what can go wrong in computer calculations and how to avert it, but also to illustrate the physical insights that some of these algorithms yield.

Topics

- Numerical instability and chaos
- Accuracy
- Nonlinear problems
- Parallel versus serial programs
- Matrix analysis of a relaxation algorithm
- Noninteger-order integration and differentiation

2.1 Introduction

2.1.1 Stable versus unstable algorithms

Computer calculations are not always correct and can sometimes go spectacularly wrong. When an algorithm is iterated, there are four possible outcomes: case 1, the error increases gradually; case 2, the error increases exponentially; case 3, chaos occurs; and case 4, the error decreases. In cases 2 and 3, the algorithm is said to be numerically unstable. More generally, a discrete algorithm formulated to solve some equation with continuous solutions (e.g., a differential equation) is said to be unstable if the algorithm yields solutions that do not correspond to those of the original equation. If, however, these extra solutions quickly decay as the iteration proceeds, the algorithm can be considered to be stable for most practical purposes.

2.1.2 Truncation and round-off error

In digital computers, a number is represented by a finite number of digits, which gives rise to truncation error (e.g., $2/3 \rightarrow 0.666$) or round-off error (e.g., $2.718 \rightarrow 2.72$). If the true value ψ_0 is input as φ_0 , the initial error is $\varepsilon_0 = \psi_0 - \varphi_0$. If ψ_0 is a physical quantity and φ_0 its measured value, then ε_0 is the measurement error.

Consider an iteration of the form

$$\psi_{t+1} = A \psi_t, \quad (2.1)$$

where A is some algorithm, and ψ_t is the true result at step $t = 0, 1, 2, \dots$. Due to truncation error, round-off error, measurement error, or a combination of

Table 2.1 Computational errors.

Step t	True value	Computed value	Error
1	$\psi_1 = A \psi_0$	$\varphi_1 = A \varphi_0$	$\varepsilon_1 = \psi_1 - \varphi_1$
2	$\psi_2 = A \psi_1$	$\varphi_2 = A \varphi_1$	$\varepsilon_2 = \psi_2 - \varphi_2$
$\vdots$			
$t+1$	$\psi_{t+1} = A \psi_t$	$\varphi_{t+1} = A \varphi_t$	$\varepsilon_{t+1} = \psi_{t+1} - \varphi_{t+1}$

these, what we actually compute is $\varphi_{t+1} = A\varphi_t$. The error at step t , $\varepsilon_t = \psi_t - \varphi_t$, arises from both the initial error, $\varepsilon_0 = \psi_0 - \varphi_0$, and errors inherent in the computation itself. Table 2.1 presents the true and computed values, and the resulting errors for step $t = 0, 1, 2, \dots, t+1$.

Note 2.1

Even if $\varepsilon_0 = 0$, which implies that $\varphi_0 = \psi_0$, ε_t for $t > 0$ does not necessarily vanish due to errors in the computational process itself.

In case 1, slowly increasing error, ε_t is a polynomial function of t , $\varepsilon_t = a_0 + a_1t + a_2t^2 + \dots$ ($a_0, a_1, \dots$ constants). $|\varepsilon_t|$ increases slowly compared with the exponential growth of case 2, where $|\varepsilon_t| \sim e^{\alpha t}$ ($\alpha > 0$). In the chaotic case 3, the error does not necessarily become infinite, but small changes in the input produce huge changes in the output, and the computation becomes unreliable after a few steps. In case 1, the error can be controlled by increasing the number of digits in the representation or by improving the measurement of φ_0 . In cases 2 and 3, ψ_t cannot be accurately computed many steps into the future. In case 4, the error actually decreases as the algorithm is iterated.

One example is worth 10,000 theorems, so let us forthwith proceed.

2.2 Bessel Recursion

A famous example of an unstable algorithm for which the error rapidly increases is the upward recursion of Bessel functions,

$$J_{n+1}(x) = \frac{2n}{x} J_n(x) - J_{n-1}(x), \quad (2.2)$$

where $J_n(x)$ denotes the n^{th} ($n = 0, \pm 1, \pm 2, \dots$) Bessel function of the first kind.

Given $J_0(x)$ and $J_1(x)$, one ought to be able to compute $J_n(x)$ for any $n > 1$. In fact, the iteration quickly diverges from the correct answer. For example, given $J_0(1) \cong 0.7652$ and $J_1(1) \cong 0.4401$, and iterating Eq. (2.2), we find the result illustrated in Fig. 2.1; the recursion is numerically unstable.

However, in downward recursion,

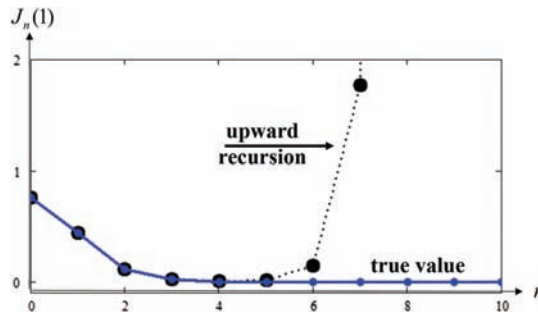


Figure 2.1 Iteration of $J_{n+1}(1) = 2nJ_n(1) - J_{n-1}(1)$ given $J_0(1)$ and $J_1(1)$. After the fourth step ($n = 5$), the error becomes large.

$$J_{n-2}(x) = \frac{2(n-1)}{x} J_{n-1}(x) - J_n(x), \quad (2.3)$$

the error decreases. Using the fact that $\lim_{n \rightarrow \infty} J_n(x) = 0$ for finite x , Bessel functions can be computed by setting $J_N(x) = 0$ for $N \gg x$ and $J_{N-1}(x) = \delta$, where δ is small. Using downward recursion yields $cJ_n(x)$, where c is a normalization constant [determined from the identities $\sum_{n=-\infty}^{\infty} J_n(x) = 1$ and $J_{-n}(x) = (-1)^n J_n(x)$]. This is an example of case 4. See Ref. 4 for further details.

2.3 Recursive Iteration

Sometimes it is possible to solve the equation $f(x) = x$ by iterating

$$x_{t+1} = f(x_t). \quad (2.4)$$

Starting with an initial guess value x_0 , we compute $x_1 = f(x_0)$, $x_2 = f(x_1)$, $\dots$. If $\lim_{t \rightarrow \infty} x_{t+1} = x_t$, then $x_\infty = \lim_{t \rightarrow \infty} x_t$ is the solution of $f(x) = x$. For example, if $f(x) = \cos x$, the iteration rapidly converges (Fig. 2.2), and we find that $x = \cos x \cong 0.7390$. The solution can be computed to arbitrary accuracy. This is an example of case 4. For any initial value x_0 , the algorithm converges and is said to be unconditionally stable. The iteration process can be represented graphically on a plot of $y = f(x)$ and $y = x$, as shown Fig. 2.3. The solution is the value of x where the two plots intersect. The lines connecting

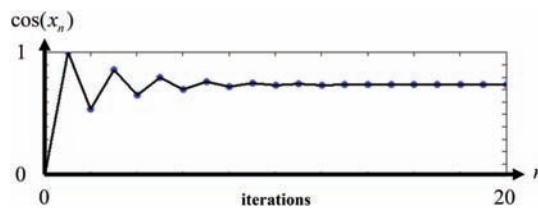


Figure 2.2 Iteration of $x_{n+1} = \cos x_n$; $x_0 = 0$.

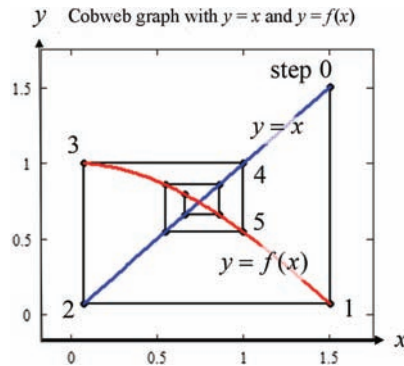


Figure 2.3 Cobweb visualization of $x_{n+1} = \cos x_n$. Initial position is $(x_0, x_0) = (1.5, 1.5)$.

points $[x_0, x_1 = f(x_0)]$, (x_1, x_1) , $[x_1, x_2 = f(x_1)]$, (x_2, x_2) , etc., form what is called the cobweb graph.

2.4 Decay Equation

We now proceed to derive several different algorithms to solve the decay equation,

$$\frac{d}{dt}\psi(t) = -\alpha\psi(t), \quad (2.5)$$

where $\alpha > 0$. Its analytic solution is

$$\psi(t) = \psi_0 e^{-\alpha t}, \quad (2.6)$$

where $\psi_0 = \psi(0)$. We now proceed to analyze the accuracy and numerical stability of several different algorithms.

2.4.1 Standard forward finite difference model

Inserting the standard forward finite difference (S-FFD) approximation $\partial_t \psi(t) \cong [\psi(t + \Delta t) - \psi(t)]/\Delta t$ into Eq. (2.5) gives

$$\psi(t + \Delta t) - \psi(t) = -\alpha \Delta t \psi(t). \quad (2.7)$$

Solving for $\psi(t + \Delta t)$ yields what is called a finite difference algorithm:

$$\psi(t + \Delta t) = (1 - \alpha \Delta t)\psi(t). \quad (2.8)$$

Let us now discretize time by taking $\Delta t = t/N$, $t = \tau\Delta t$, and $\tau = 0, 1, 2, \dots, N$. Writing $\psi(\tau\Delta t) = \psi_\tau$ for notational simplicity, Eq. (2.8) becomes

$$\psi_{\tau+1} = [1 - \alpha \Delta t] \psi_{\tau}. \quad (2.9)$$

It is easy to infer that the analytic solution of this difference equation is

$$\begin{aligned} \varphi_{\tau} &= [1 - \alpha \Delta t]^{\tau} \psi_0, \\ &= \left[1 - \alpha \frac{t}{N}\right]^N \psi_0. \end{aligned} \quad (2.10)$$

Note that throughout this section, ψ denotes the analytic solution of the original differential equation, or samples of it, and φ denotes solutions of its finite difference model.

By definition, $e^x = \lim_{N \rightarrow \infty} (1 + x/N)^N$; thus, $\lim_{N \rightarrow \infty} \varphi_{\tau} = \psi_0 e^{-\alpha t} = \psi_{\tau}$, and in the limit $\Delta t \rightarrow 0$, the numerical solution converges to the analytical solution. The error at step τ is

$$\begin{aligned} \varepsilon_{\tau} &= \psi_{\tau} - \varphi_{\tau} \\ &= e^{-\alpha \Delta t \tau} - (1 - \alpha \Delta t)^{\tau}. \end{aligned} \quad (2.11)$$

For $-1 < 1 - \alpha \Delta t < 1$, which implies that $0 < \alpha \Delta t < 2$, it is easy to see that as $\tau \rightarrow \infty$, $\varepsilon_{\tau} \rightarrow 0$; but for $|1 - \alpha \Delta t| > 1$, $|1 - \alpha \Delta t|^{\tau} = e^{\tau \ln(1 - \alpha \Delta t)}$, and hence ε_{τ} grows exponentially with the number of iterations. The condition for numerical stability is thus

$$0 < \alpha \Delta t < 2. \quad (2.12)$$

2.4.2 Standard backward finite difference model

The standard backward finite difference (S-BFD) approximation to the first derivative is $\partial_t \psi(t) \cong [\psi(t) - \psi(t - \Delta t)]/\Delta t$. Inserting this into the decay equation gives $\psi_{\tau} - \psi_{\tau-1} = -\alpha \Delta t \psi_{\tau}$, making the shift $\tau \rightarrow \tau+1$; solving for $\psi_{\tau+1}$, we obtain the difference equation

$$\psi_{\tau+1} = \frac{1}{1 + \alpha \Delta t} \psi_{\tau}. \quad (2.13)$$

The analytic solution of Eq. (2.13) is

$$\varphi_{\tau} = \frac{1}{(1 + \alpha \Delta t)^{\tau}} \psi_0. \quad (2.14)$$

Taking $\Delta t = t/N$, $t = \tau \Delta t$ ($\tau = 0, 1, 2, \dots, N$), we find that $\lim_{N \rightarrow \infty} \varphi_{\tau} = \psi_0 e^{-\alpha t}$ —the same as for the S-FFD model. The S-BFD model is, however, more stable. The condition for numerical stability is simply

$$0 < \alpha \Delta t. \quad (2.15)$$

Thus, the S-BFD algorithm can use a larger value of Δt than the S-FFD algorithm can and hence converges faster to the solution. The lesson is that convergence to the solution is not the only criterion for choosing one algorithm over another.

2.4.3 Standard central finite difference model

Although of no practical use, it is interesting to examine the standard central finite difference (S-CFD) algorithm. We cannot use $\partial_t \psi(t) \cong [\psi(t + \Delta t/2) - \psi(t - \Delta t/2)]/\Delta t$ in Eq. (2.5) because ψ_τ is known only at $t = \tau\Delta t$, but not at $t = \tau\Delta t \pm \Delta t/2$. Instead, we use the double-step expression $\partial_t \psi(t) \cong [\psi(t + \Delta t) - \psi(t - \Delta t)]/2\Delta t$. Inserting this into the decay equation gives the S-CFD model

$$\psi_{\tau+1} - \psi_{\tau-1} = -2\alpha \Delta t \psi_\tau \quad (2.16)$$

and the S-CFD algorithm

$$\psi_{\tau+1} = \psi_{\tau-1} - 2\alpha \Delta t \psi_\tau. \quad (2.17)$$

The analytic solution of Eq. (2.17) can be found by postulating a solution of the form $\varphi_\tau = \lambda^\tau$. Substituting this into Eq. (2.17) gives

$$\lambda^2 + (2\alpha\Delta t)\lambda - 1 = 0, \quad (2.18)$$

which has the solutions $\lambda = \lambda_\pm$, where

$$\lambda_\pm = -\alpha\Delta t \pm \sqrt{1 + (\alpha\Delta t)^2}. \quad (2.19)$$

The general solution is the linear combination

$$\varphi_\tau = a_+ \lambda_+^\tau + a_- \lambda_-^\tau, \quad (2.20)$$

where $a_\pm$ are constants.

It is easy to see that $|\lambda_+| < 1$ and $|\lambda_-| > 1$ for all $\Delta t > 0$ and $\alpha > 0$. Since the solution of the decay equation is a falling exponential, and one of the solutions of the difference equation [Eq. (2.16)] is a rising exponential, the S-CFD algorithm is numerically unstable.

For educational purposes, it is interesting to carry on with the analysis. The $a_\pm$ values are determined by the initial conditions

$$\psi_0 = a_+ + a_-, \quad (2.21a)$$

$$\psi_1 = a_+ \lambda_+ + a_- \lambda_-, \quad (2.21b)$$

and we find that

$$a_{\pm} = \frac{\pm \psi_1 \mp \psi_0 \lambda_{\mp}}{\lambda_+ - \lambda_-}. \quad (2.22)$$

Taking $\psi_0 = 1$, the analytic solution of the decay equation gives $\psi_1 = e^{-\alpha \Delta t}$, and we obtain

$$a_{\pm} = \frac{1}{2} \left[1 \pm \frac{\alpha \Delta t + e^{-\alpha \Delta t}}{\sqrt{1 + (\alpha \Delta t)^2}} \right]. \quad (2.23)$$

Although $\lim_{\Delta t \rightarrow 0} a_- = 0$, there is no value of $\Delta t > 0$ such that $a_- = 0$. The error of the S-SCD algorithm is $\varepsilon_{\tau} \sim (-1)^{\tau} |\lambda_-|^{\tau} - \psi_0 e^{-\alpha \tau \Delta t}$, and it oscillates and grows exponentially as the iteration proceeds. The S-CFD algorithm is said to be unconditionally unstable because it is unstable for all $\Delta t > 0$. This is despite the fact that the solution of the difference equation [Eq. (2.17)] converges to the solution of the decay equation in the limit $\Delta t \rightarrow 0$, $\lim_{\Delta t \rightarrow 0} \varphi_{\tau} = \psi_0 e^{-\alpha \tau \Delta t} = \psi_{\tau}$.

In Fig. 2.4, the S-CFD algorithm is compared with the analytic solution for $\alpha \Delta t = 0.04$, which implies that $\lambda_+ = 0.961$, $\lambda_- = -1.041$, $a_+ = 0.999995$, and $a_- = 5.116 \times 10^{-6}$. Up to about 150 iterations $|a_- \lambda_-^{\tau}|$ is small, but afterwards its amplitude rapidly increases.

Note 2.2

The S-CFD model fundamentally differs from the S-FFD model. The former uses second-order FDs and requires two initial conditions to define a solution, while the latter uses first-order FDs and requires one initial condition. Mickens⁵ has shown that when the order of a FD model is greater than that of the original differential equation, spurious solutions and numerical instability can arise.

Although $d\varphi(t)/dt = 0$ and $d^2\varphi(t)/dt^2 = 0$ share a subset of solutions, the latter has solutions that are very different from the former. In the same way, a second-order FD model of a first-order differential equation has extra solutions that have no relationship to those of the original differential equation.

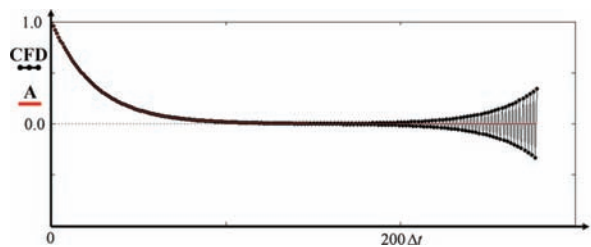


Figure 2.4 Standard CFD algorithm versus the analytic solution (A) of the decay equation for $\alpha \Delta t = 0.04$.

2.4.4 Nonstandard central finite difference model

Although we expect it to be numerically unstable, it is nonetheless interesting to examine the nonstandard central finite difference (NS-CFD) model. An exact NS-CFD expression for the derivative of $\psi = e^{-\alpha t}$ is

$$\frac{\psi(t + \Delta t) - \psi(t - \Delta t)}{-2 \sinh(\alpha \Delta t)/\alpha} = \partial_t \psi(t). \quad (2.24)$$

Inserting Eq. (2.24) into the decay equation and solving for $\psi(t + \Delta t)$, we obtain the NS-CFD algorithm

$$\psi_{\tau+1} = \psi_{\tau-1} - 2 \sinh(\alpha \Delta t) \psi_{\tau}. \quad (2.25)$$

Repeating the steps in Eqs. (2.20)–(2.23) with the substitution $\alpha \Delta t \rightarrow \sinh(\alpha \Delta t)$, and using the identity $\cosh^2 x - \sinh^2 x = 1$, we find that

$$\begin{aligned} \lambda_+ &= -\sinh(\alpha \Delta t) + \cosh(\alpha \Delta t) \\ &= e^{-\alpha \Delta t}, \end{aligned} \quad (2.26a)$$

$$\begin{aligned} \lambda_- &= -\sinh(\alpha \Delta t) - \cosh(\alpha \Delta t) \\ &= -e^{+\alpha \Delta t}, \end{aligned} \quad (2.26b)$$

$$a_+ = 1, \quad (2.27a)$$

$$a_- = 0. \quad (2.27b)$$

The analytic solution of the difference equation [Eq. (2.25)] is thus

$$\phi_{\tau} = e^{-\alpha \tau \Delta t} + 0 \cdot (-1)^{\tau} e^{\alpha \tau \Delta t}. \quad (2.28)$$

Mathematically, the NS-CFD model is exact.

Because the coefficient of the rising exponential is $a_- = 0$, we might hope that the NS-CFD algorithm is numerically stable. It is not. Due to round-off and truncation errors in the computational process, at some step in the computation, $e^{-\alpha \tau \Delta t}$ becomes $e^{-\alpha \tau \Delta t} + \delta(-1)^{\tau} e^{\alpha \tau \Delta t}$ ($\delta \neq 0$). However small $|\delta|$ might be, the error now rises exponentially. But the divergence of the NS-CFD calculation does occur later than that of the S-CFD calculation. For the same parameters as were used in Fig. 2.4, the iteration of the NS-CFD algorithm starts to noticeably diverge after about 800 steps (compared with 150 steps for the S-CFD algorithm).

The lesson is that even when numerical instability cannot be eliminated, it may sometimes be possible to delay it long enough to obtain a useable result. See Program MC2.1 for an implementation and comparison of different FD algorithms to solve the decay equation.

2.4.5 Nonstandard forward finite difference model

Finally, let us develop an exact and stable algorithm to solve the decay equation. $\partial_t e^{-\alpha t} = d_t^f e^{-\alpha t}/s$, exactly, where $s = (1 - e^{-\alpha \Delta t})/\alpha$, and $d_t^f \psi(t) = \psi(t + \Delta t) - \psi(t)$. Replacing $\alpha \Delta t$ by $(1 - e^{-\alpha \Delta t})$ in the S-FFD model of Eq. (2.7) yields the NS-FFD algorithm

$$\psi_{\tau+1} = e^{-\alpha \Delta t} \psi_{\tau}. \quad (2.29)$$

This algorithm is both exact and unconditionally stable. Also, it applies to the case where $\alpha < 0$, i.e., a growth equation—see below.

2.5 Malthus Model of Population Growth

Replacing $-\alpha \rightarrow +\alpha$ ($\alpha > 0$) in Eq. (2.5) gives the model of population growth proposed by Thomas Malthus in 1798:⁵

$$\frac{d}{dt} \psi(t) = \alpha \psi(t). \quad (2.30)$$

Its analytic solution is

$$\psi(t) = \psi_0 e^{\alpha t}. \quad (2.31)$$

The standard forward finite difference (S-FFD) model is

$$\psi_{\tau+1} = (1 + \alpha \Delta t) \psi_{\tau}, \quad (2.32)$$

and its analytical solution is

$$\begin{aligned} \varphi_{\tau} &= [1 + \alpha \Delta t]^{\tau} \psi_{\tau} \\ &= e^{\tau \ln(1 + \alpha \Delta t)}. \end{aligned} \quad (2.33)$$

Its error is

$$\begin{aligned} \varepsilon_{\tau} &= \psi_{\tau} - \varphi_{\tau} \\ &= e^{\tau \alpha \Delta t} - e^{\tau \ln(1 + \alpha \Delta t)}. \end{aligned} \quad (2.34)$$

The S-FFD algorithm is numerically stable because it has no spurious solutions.

An analysis of the S-CFD model of the Malthus equation [Eq. (2.30)] shows that this model is technically unstable because one of its solutions is a falling exponential (which is not a solution of the original differential equation). However, this extra solution vanishes as the iteration proceeds, so the S-CFD model can be considered stable for practical purposes. The CFD models are of little interest here, so we omit their analyses.

An exact, unconditionally stable NS-FFD algorithm to solve the Malthus equation is derived with the substitution of $-\alpha \rightarrow +\alpha$ into Eq. (2.29) to obtain $\psi_{\tau+1} = e^{\alpha \Delta t} \psi_{\tau}$.

2.6 Finite Difference Models of Nonlinear Differential Equations

Malthus himself realized that indefinite exponential growth of a real population is impossible, and he predicted that war, disease, and famine would stop it. The simplest model in which growth decreases with increasing population is the Verhulst model⁶ (often called the logistic equation), given by

$$\frac{d}{dt} \psi(t) = \alpha \left[1 - \frac{\psi(t)}{M} \right] \psi(t), \quad (2.35)$$

where M is the maximum sustainable population. Without loss of generality, we take $M = 1$, and Eq. (2.35) becomes

$$\frac{d}{dt} \psi(t) = \alpha [1 - \psi(t)] \psi(t). \quad (2.36)$$

The analytical solution to Eq. (2.36) is

$$\psi(t) = \frac{\psi_0 e^{\alpha t}}{1 + \psi_0 (e^{\alpha t} - 1)}. \quad (2.37)$$

Usually, it is difficult to find good numerical solutions for nonlinear equations, so it is interesting to construct finite difference solutions of the logistic equation that can be compared with its analytic solution.

2.6.1 Standard forward finite difference model

The S-FFD algorithm is a good example of what can go wrong with numerical solutions of nonlinear differential equations. In fact, the S-FFD algorithm has been a topic of research, not as a solution of the logistic equation, but as an example of deterministic chaos.⁷

Inserting the S-FFD approximation $\partial_t \psi(t) \cong [\psi(t + \Delta t) - \psi(t)]/\Delta t$ into Eq. (2.36), we obtain the S-FFD algorithm

$$\psi_{\tau+1} = \psi_{\tau} + \alpha \Delta t (1 - \psi_{\tau}) \psi_{\tau}. \quad (2.38)$$

Obviously, $\varphi_{\tau} = 1$ is a solution of Eq. (2.38). It is said to have period = 1 because $\varphi_{\tau+1} = \varphi_{\tau}$. Since the logistic equation models positive quantities, we consider only positive solutions (for negative solutions, the growth rate is always positive).

Next, let us seek solutions of period = 2. Iterating Eq. (2.38) once again and setting $\varphi_{\tau+2} = \varphi_{\tau}$, we obtain

$$0 = \bar{\alpha} \varphi_{\tau} (\varphi_{\tau} - 1) [(\bar{\alpha}^2 \varphi_{\tau}^2 - \bar{\alpha}(2 + \bar{\alpha})\varphi_{\tau} + (2 + \bar{\alpha}))], \quad (2.39)$$

where, for brevity, we write $\bar{\alpha} = \alpha \Delta t$. Solving for the $\varphi_{\tau} \neq 0$ and $\varphi_{\tau} \neq 1$ roots, we find that $\varphi_{\tau} = r_{\pm}$, where

$$r_{\pm} = \frac{(\bar{\alpha} + 2) \pm \sqrt{(\bar{\alpha} + 2)(\bar{\alpha} - 2)}}{2\bar{\alpha}}. \quad (2.40)$$

For $\bar{\alpha} > 2$, the $r_{\pm}$ values are real, and it is easy to show that if $\varphi_{\tau} = r_{\pm}$, then $\varphi_{\tau+1} = r_{\mp}$. This tells us that φ_{τ} oscillates between r_{+} and r_{-} with period = 2. Since the original logistic equation [Eq. (2.36)] has no oscillatory solutions, the S-FFD algorithm is numerically unstable for $\bar{\alpha} > 2$. We might conclude that it is stable for $0 < \bar{\alpha} < 2$, but iteration of Eq. (2.38) shows that there are transient oscillations that become larger and decay more slowly as $\bar{\alpha} \rightarrow 2$. For $\bar{\alpha} \geq 3$, the iteration yields solutions $\varphi_{\tau} \leq 0$ that are irrelevant for our purposes.

Interesting behavior occurs in the range $2 < \bar{\alpha} < 3$. As $\bar{\alpha}$ increases beyond 2, the oscillation period of φ_{τ} rises from $1 \rightarrow 2 \rightarrow 4 \rightarrow \dots \rightarrow 2^n$ ($n = 0, 1, 2, \dots$). This process is called period doubling or bifurcation. (The higher-order period solutions, $\varphi_{\tau+2n} = \varphi_{\tau}$, are difficult or impossible to find analytically.) During period = 2^n , φ_{τ} passes through 2^n different values. Bifurcation continues as $\bar{\alpha} \rightarrow \bar{\alpha}^* \cong 2.667$ and $n \rightarrow \infty$, as shown in Fig. 2.5. The value of $\bar{\alpha}^*$ can be estimated using Feigenbaum's theorem.⁸

At $\bar{\alpha} = \bar{\alpha}^*$, the period is infinite, and φ_{τ} takes an infinite number of values. Since an infinite period implies aperiodicity, φ_{τ} never returns to its initial value. The calculation is extremely sensitive to small perturbations (such as those that arise from truncation or round-off error), so the long-term behavior of φ_{τ} is not computable. This is the defining characteristic of what is called deterministic chaos. Given φ_0 , Eq. (2.38) provides, in principle, a deterministic

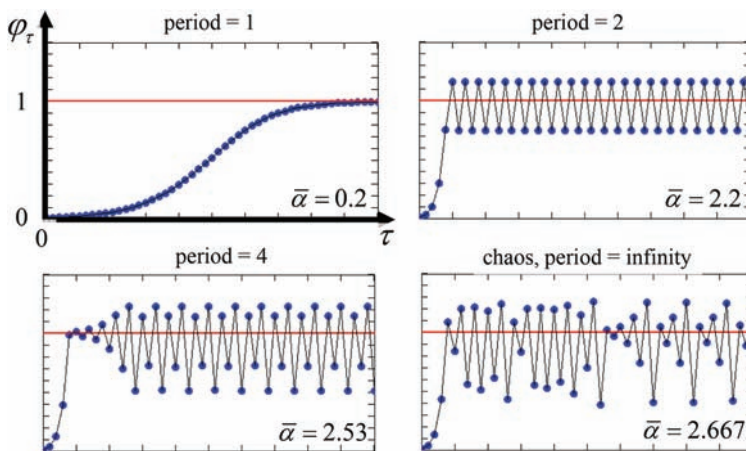


Figure 2.5 Bifurcation to chaos as $\bar{\alpha} \rightarrow \bar{\alpha}^*$ in the iteration of the S-FFD algorithm.

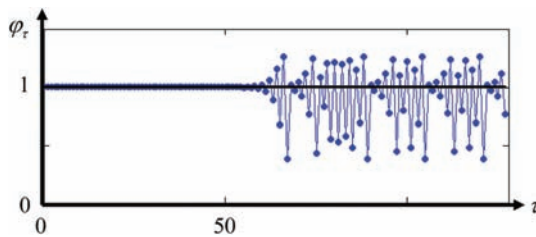


Figure 2.6 Instability and extreme sensitivity to perturbation of the S-FFD algorithm; $\varphi_0 = 1 + 10^{-15}$ and $\bar{\alpha} = 2.667$.

formula to compute all subsequent values of φ_τ , but, in fact, they are not (accurately) computable. Phenomena of this sort were first reported by Lorenz⁹ and are not limited to the S-FFD model of the logistic equation.

Equation (2.38) tells us that for $\varphi_0 = 1$, $\varphi_1 = \varphi_2 = \dots = 1$ for any value of $\bar{\alpha}$, but when we iterate the S-FFD algorithm using $\bar{\alpha} = 2.667$ and $\varphi_0 = 1 + 10^{-15}$, this algorithm displays strong oscillations after about 50 iterations, as seen in Fig. 2.6. (For $\psi_0 = 1 + 10^{-15}$, the analytic solution [Eq. (2.37)] very quickly relaxes to $\psi = 1$ for $t > 0$.)

Deterministic chaos is a common feature of many systems, including the Solar System. Two-body orbits are stable; although three-body systems are, in principle, deterministic, they display chaotic behavior.

Note 2.3

Defining $\mu = 1 + \alpha\Delta t$ and $y_\tau = [(\mu - 1)/\mu]\psi_\tau$ gives what is called the standard form of the logistic equation:

$$y_{\tau+1} = \mu y_\tau (1 - y_\tau). \quad (2.41)$$

This is the form most often treated in the literature and is sometimes called the logistic equation.

The arrow of time. In the chaotic state, we cannot compute the future from the present, but can we compute the past given the present? Making the replacement $\tau \rightarrow \tau - 1$ in Eq. (2.41), we obtain $y_\tau = \mu y_{\tau-1} (1 - y_{\tau-1})$. Solving for $y_{\tau-1}$, we find that $y_{\tau-1} = 1/2 \pm \sqrt{\mu^2 - 4\mu y_\tau}/2\mu$. Except for the special case where $y_\tau = 1/2$ and $\mu = 4y_\tau$, given y_τ , there are two possible values of $y_{\tau-1}$. Going back one more step, given y_τ , there are four possible values of $y_{\tau-2}$. In general, there are 2^n possible values of $y_{\tau-n}$ that give y_τ . Thus, when we try to reconstruct the past from the present, the farther back we go the more uncertain it becomes. This fits with common observation. Imagine a crime scene. The longer the elapsed time since the discovery of the crime the more difficult it is to find the criminal. Most biological processes are irreversible,

and we cannot go back to the past. The discrete logistic equation tells us, heuristically, why this is so.

2.6.2 Nonstandard forward finite difference model

We now proceed to construct a stable and accurate algorithm to actually solve the logistic equation using the nonstandard methodology.¹⁰

A general rule is that nonlinear terms such as $\psi(t)^2$ in Eq. (2.36) must be modeled nonlocally; for example,

$$\psi(t)^2 \rightarrow \psi(t)\psi(t + \Delta t). \quad (2.42)$$

Let us pretend that we do not know the analytic solution of Eq. (2.36) but guess that it contains an exponential. An exact NS-FFD expression for the derivative of $\psi(t) = e^{\alpha t}$ is

$$\alpha \frac{\psi(t + \Delta t) - \psi(t)}{(e^{\alpha \Delta t} - 1)} = \partial_t e^{\alpha t}. \quad (2.43)$$

Inserting Eqs. (2.42) and (2.43) into the Verhulst equation [Eq. (2.36)], we obtain its NS-FFD model,

$$\psi_{\tau+1} - \psi_{\tau} = (e^{\alpha \Delta t} - 1)(\psi_{\tau} - \psi_{\tau}\psi_{\tau+1}) \quad (2.44)$$

and the NS-FFD algorithm,

$$\varphi_{\tau+1} = \frac{e^{\alpha \Delta t} \varphi_{\tau}}{[1 + (e^{\alpha \Delta t} - 1) \varphi_{\tau}]}. \quad (2.45)$$

Figure 2.7 compares the S-FFD [Eq. (2.38)] and NS-FFD [Eq. (2.45)] algorithms with the analytic solution in Eq. (2.37) for $\alpha \Delta t = 2.5$. As we can see, the NS-FFD algorithm gives a very accurate result and is stable for all $\alpha \Delta t > 0$. NS models for nonlinear differential equations are further developed in Ref. 11.

We do not cover nonlinear optics in this book, but we note that nonstandard techniques introduced here can improve the accuracy of calculations of the properties of nonlinear materials. For example, in the

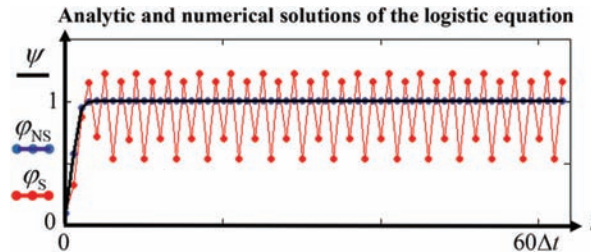


Figure 2.7 Comparison of the NS-FFD and S-FFD calculations with the analytic solution of the differential logistic equation for $\alpha \Delta t = 2.5$.

Pockels effect, a factor of E^2 (E is the electric field) appears in Maxwell's equations. We plan to develop this topic in later publications.

2.7 Relaxation Algorithm for the Laplace Equation and Poisson's Equation

2.7.1 Basic relaxation algorithm

Poisson's equation is given by

$$\nabla^2 \psi(\mathbf{x}) = \rho(\mathbf{x}), \quad (2.46)$$

where ρ is some function, and $\mathbf{x} = (x, y, z)$. When $\rho = 0$, Poisson's equation is called the Laplace equation. In electrostatics, ψ represents the electric field potential and ρ the charge density. The Newtonian gravitational potential is also described by Poisson's equation.

Usually, the value of ψ is specified on the boundaries of some region. For example, when a charge distribution is located inside a grounded, perfectly conducting shell, then $\psi = 0$ on the shell. In the case of complicated nonsymmetrical boundaries, Poisson's equation can be difficult or impossible to solve analytically.

The relaxation algorithm is not only an effective numerical method, but it also yields insight into the difference between parallel and serial computing, and has interesting physical and mathematical interpretations as well.

For simplicity, we first examine Poisson's equation in one dimension, where it reduces to

$$\partial_x^2 \psi(x) = \rho(x). \quad (2.47)$$

A FD model of Eq. (2.47) is

$$d_x^2 \psi(x) = h \rho(x), \quad (2.48)$$

where $d_x^2 \psi(x) = \psi(x+h) + \psi(x-h) - 2\psi(x)$ (see Chapter 1). Solving for $\psi(x)$, we find that

$$\psi(x) = \frac{\psi(x+h) + \psi(x-h)}{2} - \frac{1}{2} h^2 \rho(x). \quad (2.49)$$

At first sight, Eq. (2.49) may seem of little use because ψ is unknown. But when boundary conditions are specified, the values of ψ on the boundaries determine ψ in the interior.

Take the domain of ψ to be $0 \leq x \leq b$, and let $b = Nh$, where $N > 0$ is an integer. Let $x = \chi h$, where $0 \leq \chi \leq N$ is an integer, and define $\psi_\chi = \psi(\chi h)$ and $\rho_\chi = \rho(\chi h)$. On the boundary B , $\chi = 0$ or $\chi = N$, and in the interior I , $1 < \chi < N - 1$. Then Eq. (2.49) becomes

$$\psi_\chi = \frac{\psi_{\chi-1} + \psi_{\chi+1}}{2} - \frac{1}{2}h^2\rho_\chi \quad (2.50)$$

for $\chi \in I$. This is the basic relaxation algorithm. This algorithm can be iterated and, as we will show, converges to the solution of Poisson's 1D equation.

Let φ_χ^τ be the computed value of ψ_χ at iteration step τ , and let φ_χ^0 be a vector of guess values of ψ_χ , or random or arbitrary numbers for $\chi \in I$. On the boundary, $\varphi_0^0 = \psi_0$ and $\varphi_N^0 = \psi_N$, which are specified by the boundary conditions. The relaxation algorithm now becomes

$$\varphi_\chi^{\tau+1} = \frac{\varphi_{\chi-1}^\tau + \varphi_{\chi+1}^\tau}{2} - \frac{1}{2}h^2\rho_\chi \quad \text{for } \chi \in I, \quad (2.51a)$$

$$\varphi_\chi^{\tau+1} = \varphi_\chi^\tau \quad \text{for } \chi \in B. \quad (2.51b)$$

Note that this is not the most efficient form of the relaxation algorithm. A form that converges more rapidly is given in Section 2.7.5.

Defining the relaxation operator $\mathbf{R}$ by

$$\begin{aligned} (\mathbf{R}\psi)_\chi &= \frac{\psi_{\chi+1} + \psi_{\chi-1}}{2} \quad \text{for } \chi \in I, \\ (\mathbf{R}\psi)_\chi &= \psi_\chi \quad \text{for } \chi \in B, \end{aligned} \quad (2.52)$$

the FD model [Eq. (2.48)] of Poisson's 1D equation becomes

$$\psi = \mathbf{R}\psi - \frac{1}{2}h^2\mathbf{J}\rho, \quad (2.53)$$

where

$$\begin{aligned} (\mathbf{J}\rho)_\chi &= \rho_\chi \quad \text{for } \chi \in I, \\ (\mathbf{J}\rho)_\chi &= 0 \quad \text{for } \chi \in B. \end{aligned} \quad (2.54)$$

$\mathbf{J}$ sets the values of ρ to zero on the boundary and leaves the interior points unchanged so that the function ρ does not affect the boundary values of ψ in Eq. (2.52).

The relaxation algorithm [Eq. (2.50)] can now be compactly expressed as

$$\varphi^{\tau+1} = \mathbf{R}\varphi^\tau - \frac{1}{2}h^2\mathbf{J}\rho, \quad (2.55)$$

where, $\tau = 0, 1, \dots$. Iterating Eq. (2.55) from $\tau = 0$, we find that

$$\varphi^\tau = \mathbf{R}^\tau \varphi^0 - \frac{1}{2}h^2\mathbf{S}^\tau, \quad (2.56)$$

where $\mathbf{R}^\tau$ denotes τ applications of $\mathbf{R}$, and $\mathbf{S}^\tau = \sum_{m=0}^{\tau-1} \mathbf{R}^m \mathbf{J}$.

Defining $\mathbf{R}^\infty = \lim_{\tau \rightarrow \infty} \mathbf{R}^\tau$ and $\mathbf{S}^\infty = \lim_{\tau \rightarrow \infty} \mathbf{S}^\tau$, if both limits exist, then in the limit $\tau \rightarrow \infty$, Eq. (2.56) converges to

$$\varphi^\infty = \mathbf{R}^\infty \varphi^0 - \frac{1}{2} h^2 \mathbf{S}^\infty \rho, \quad (2.57)$$

which is a solution of Eq. (2.53) for arbitrary φ^0 because $\mathbf{R}\mathbf{R}^\infty = \mathbf{R}^\infty \mathbf{R} = \mathbf{R}^\infty$, and $\mathbf{R}\mathbf{S}^\infty = \mathbf{S}^\infty - \mathbf{R}\mathbf{J}$. In the case where $\rho = 0$ (Laplace equation), it is interesting to note that φ^∞ is a solution, regardless of the value of h .

2.7.2 Relaxation and diffusion

We can interpret φ_χ^τ as the discretized form of a space-time function $\varphi(x, t)$, where $x = \chi h$, and $t = \tau \Delta t$. Similarly, $\rho(x) \rightarrow (x, t)$ and $\rho_\chi^\tau = \rho(\chi h, \tau \Delta t)$. Subtracting φ_χ^τ from both sides of Eq. (2.51), we obtain

$$\varphi_\chi^{\tau+1} - \varphi_\chi^\tau = \frac{\varphi_{\chi-1}^\tau + \varphi_{\chi+1}^\tau - 2\varphi_\chi^\tau}{2} - \frac{1}{2} h^2 \rho_\chi^\tau, \quad (2.58)$$

which is equivalent to the difference equation

$$\varphi(x, t + \Delta t) - \varphi(x, t) = \frac{1}{2} [\varphi(x + h, t) + \varphi(x - h, t) - 2\varphi(x, t)] - \frac{1}{2} h^2 \rho(x). \quad (2.59)$$

Equation (2.59) can be rewritten as

$$\frac{\varphi(x, t + \Delta t) - \varphi(x, t)}{\Delta t} = \frac{1}{2} \frac{h^2}{\Delta t} \left[\frac{\varphi(x + h, t) + \varphi(x - h, t) - 2\varphi(x, t)}{h^2} - \rho(x, t) \right] \quad (2.60)$$

or

$$\frac{d_t^f(x, t)}{\Delta t} = \mu \left[\frac{d_x^2}{h^2} - \rho(x, t) \right], \quad (2.61)$$

where $\mu = h^2/2\Delta t$, and d_t^f is the FFD operator (see Chapter 1). This difference equation is a FD model of the inhomogeneous diffusion equation,

$$\partial_t \varphi(x, t) = \mu \partial_x^2 \varphi(x, t) - \rho(x, t), \quad (2.62)$$

where μ is the diffusion coefficient, and ρ , redefined as $\rho \rightarrow \mu\rho$, is a source term. When $\rho = 0$, this becomes the homogeneous diffusion equation:

$$\partial_t \varphi(x, t) = \mu \partial_x^2 \varphi(x, t). \quad (2.63)$$

If $\varphi(x, t)$ represents the temperature at position x at time t , then Eq. (2.63) is called the heat equation. In this case, $\varphi(x, 0) = \varphi_\chi^0$ is the initial temperature

distribution, and the heat equation describes how this distribution evolves in time. The boundary conditions model a temperature distribution that is constant on the boundaries of the domain of φ . The inhomogeneous term $\rho \neq 0$ is a heat source distribution.

The solution of the heat equation [Eq. (2.63)] at $t \rightarrow \infty$ is the same as that of the Laplace equation, $\partial_x^2 \varphi(x) = 0$. In fact, one says that the temperature distribution *relaxes* to its equilibrium distribution. When $\rho = \rho(x)$ (no time dependence), the $t \rightarrow \infty$ solution of the heat equation with a source [Eq. (2.56)] is same as the solution of Poisson's equation.

These considerations apply in two and three dimensions, where the homogeneous heat equation becomes

$$\partial_t \varphi(\mathbf{x}, t) = \mu \nabla^2 \varphi(\mathbf{x}, t), \quad (2.64)$$

where $\mathbf{x} = (x, y, z)$.

The FD model of the heat equation becomes

$$\varphi(\mathbf{x}, t + \Delta t) - \varphi(\mathbf{x}, t) = \mu \frac{\Delta t}{h^2} \mathbf{d}^2(\mathbf{x}, t), \quad (2.65)$$

where $\mathbf{d}^2 = d_x^2 + d_y^2 + d_z^2$ (see Section 1.3). Solving for $\varphi(\mathbf{x}, t + \Delta t)$, we obtain an FDTD algorithm:

$$\varphi(\mathbf{x}, t + \Delta t) = \varphi(\mathbf{x}, t) + \mu \frac{\Delta t}{h^2} \mathbf{d}^2(\mathbf{x}, t). \quad (2.66)$$

Note 2.4

The term FDTD often refers to the methodology used for solving Maxwell's equations or the wave equation. We use it here to emphasize that the FDTD methodology is applicable to many other problems as well.

FDTD is not the most computationally efficient way to solve the heat equation; the Crank–Nicolson method gives much faster convergence.¹² The important lesson here is the equivalence of the relaxation algorithm to the FDTD algorithm for the diffusion equation.

2.7.3 Analytical solutions

Let us now proceed to develop program implementations of the relaxation algorithm. Exactly how it is programmed greatly affects the speed of convergence.

In order to evaluate the accuracy and convergence speed of our programs, let us first find the analytic solution of Poisson's equation [Eq. (2.47)]. Taking

the boundary values to be $\psi(0)=\psi_0$ and $\psi(b)=\psi_N$, twice integrating Eq. (2.47) and enforcing the boundary conditions, we obtain

$$\psi(x) = [\psi_N - \psi_0 - I(b)] \frac{x}{b} + I(x), \quad (2.67)$$

where

$$\begin{aligned} I(x) &= \int_0^x dx' \int_0^{x'} dx'' \rho(x'') \\ &= \int_0^x dx' (x - x') f(x'). \end{aligned} \quad (2.68)$$

See Appendix 2.2 for further discussion of the integration in Eq. (2.68) and its generalization to higher- and noninteger-order integration.

In discretized form, Eq. (2.67) becomes

$$\psi_\chi = (\psi_N - \psi_0 - I_N) \frac{\chi}{N} + I_\chi, \quad (2.69)$$

where $I_\chi = I(\chi h)$.

2.7.4 Parallel versus serial computing

There are two separate and unequal basic implementations of the relaxation algorithm: serial update and parallel update, which are given below in pseudocode (PC).

Let ϕ^τ be the approximation to ψ at iteration step τ , where ψ is the analytic solution given by Eq. (2.63). We hope that $\lim_{\tau \rightarrow \infty} \phi^\tau = \psi$. Of course, we want the error to be small after as few iterations as possible.

The literal interpretation of the relaxation process of Eq. (2.49) is the parallel relaxation algorithm. In parallel relaxation, all of the ϕ_χ^τ values are updated simultaneously.

Program PC2.1 Parallel Relaxation (serial programming language, pseudocode)

```

1.   initialize  $\phi$ , define  $\rho$ 
2.   do for  $\tau=1, 2, \dots, M$       ! iteration loop
3.     do for  $\chi=1, 2, \dots, N-1$   ! update loop
4.        $y_\chi = \phi_\chi$ 
5.        $\phi_\chi = \frac{1}{2}(y_{\chi-1} + y_{\chi+1}) - \frac{1}{2}h^2\rho_\chi$ 
6.     end do
7.   end do
```

In a programming language such as Parallel FORTRAN, a relaxation program is shown in Program PC2.2.

Program PC2.2

Parallel Relaxation (parallel programming language, pseudocode)

1. initialize φ , define ρ
 2. do for $\tau=1, 2, \dots, M$
 3. $= \frac{1}{2}[\text{cshift}(\varphi, \text{up}) + \text{cshift}(\varphi, \text{down})] - \frac{1}{2}h^2\rho$
 4. $\varphi_0 = \psi_0$! enforce boundary conditions
 5. $\varphi_N = \psi_N$
 6. end do
-

cshift is the circular shift function defined by $\text{cshift}(\varphi, \text{up})|_{\chi} = \varphi_{\chi-1}$ for $\chi = 1, 2, \dots, N$ and $\text{cshift}(\varphi, \text{up})|_0 = \varphi_N$, while $\text{cshift}(\varphi, \text{down})|_{\chi} = \varphi_{\chi+1}$, for $\chi = 0, 1, \dots, N-1$ and $\text{cshift}(\varphi, \text{down})|_N = \varphi_0$.

In component form, the parallel program is equivalent to

$$\varphi_{\chi}^{\tau+1} = \frac{1}{2}(\varphi_{\chi-1}^{\tau} + \varphi_{\chi+1}^{\tau}) - \frac{1}{2}h^2\rho_{\chi} \quad (2.70)$$

for $\chi \in I$, while $\varphi_{\chi}^{\tau+1} = \varphi_{\chi}^{\tau}$ for $\chi \in B$.

In a serial program, the elements of φ^{τ} are updated sequentially, as shown in Program PC2.3.

Program PC2.3

Forward Serial Relaxation Program (serial programming language, pseudocode)

1. initialize φ , define ρ
 2. do for $\tau=1, 2, \dots, M$! iteration loop
 3. do for $\chi=1, 2, \dots, N-1$! update loop
 4. $\varphi_{\chi} = \frac{1}{2}(\varphi_{\chi-1} + \varphi_{\chi+1}) - \frac{1}{2}h^2\rho_{\chi}$
 5. end do
 6. end do
-

In this program, $\chi=1, 2, \dots, N-1$ (hence, the term “forward”), so $\varphi_{\chi-1}$ is updated before φ_{χ} . This forward serial relaxation program is thus equivalent to

$$\varphi_{\chi}^{\tau+1} = \frac{1}{2}(\varphi_{\chi-1}^{\tau+1} + \varphi_{\chi+1}^{\tau}) - \frac{1}{2}h^2\rho_{\chi} \quad (2.71)$$

for $\chi \in I$; for $\chi \in B$, $\varphi_{\chi}^{\tau+1} = \varphi_{\chi}^{\tau}$. Obviously, Eq. (2.71) differs from the FD model of Poisson’s equation given by Eq. (2.51).

Reversing the loop in line three of the forward serial program yields the backward serial program,

$$\varphi_i^{\tau+1} = \frac{1}{2}(\varphi_{i-1}^{\tau} + \varphi_{i+1}^{\tau+1}) - \frac{1}{2}h^2\rho_x, \quad (2.72)$$

where $i = N - 1, N - 2, \dots, 1$.

The rate of convergence of serial programs can depend on the details of the boundary conditions and on φ^0 , itself. For example, if $\varphi_0 = 0$ and $\psi_N \neq 0$, and $\varphi_i^0 = 0$ for $i \in \{I\}$, then the $i = 1, 2, \dots, N - 1$ loop is faster because the value of ψ_N affects the calculation starting with the first iteration.

Although parallel programs often run faster than serial programs, the serial relaxation program for Poisson's and the Laplace equations converges faster than that of the parallel program, but both converge rather slowly. The convergence speed can be greatly improved by using what is called over-relaxation.

2.7.5 Over-relaxation

Defining $\Delta\varphi_x^{\tau} = \varphi_x^{\tau+1} - \varphi_x^{\tau}$, $\varphi_x^{\tau+1} = \varphi_x^{\tau} + \Delta\varphi_x^{\tau}$. Let us try to speed up the convergence of the serial relaxation program by replacing $\Delta\varphi_x^{\tau}$ with $(1 + \eta)\Delta\varphi_x^{\tau}$, where $\eta \geq 0$ is a parameter. Thus,

$$\varphi_x^{\tau+1} = \varphi_x^{\tau} + (1 + \eta)\Delta\varphi_x^{\tau}. \quad (2.73)$$

Program PC2.4

Serial Over-Relaxation Program (serial programming language, pseudocode)

1. initialize φ , define ρ , define over-relaxation parameter = η
 2. do for $\tau = 1, 2, \dots, M$! iteration loop
 3. do for $\chi = 1, 2, \dots, N-1$! update loop
 4. $y_{\chi} = \varphi_{\chi}$! current $\varphi = y$
 5. $\varphi_{\chi} = \frac{1}{2}(\varphi_{\chi-1} + \varphi_{\chi+1}) - \frac{1}{2}h^2\rho_{\chi}$! updated φ
 6. $\Delta\varphi_{\chi} = \varphi_{\chi} - y_{\chi}$
 7. $\varphi_{\chi} = y_{\chi} + (1 + \eta)\Delta\varphi_{\chi}$
 8. end do
 9. end do
-

From Eq. (2.71), $\Delta\varphi_x^{\tau} = (\varphi_{x-1}^{\tau+1} + \varphi_{x+1}^{\tau})/2 - \varphi_x^{\tau} - h^2\rho_x/2$; hence, the forward serial over-relaxation program computes

$$\varphi_x^{\tau+1} = \frac{1}{2}(1 + \eta)(\varphi_{x-1}^{\tau+1} + \varphi_{x+1}^{\tau}) - \eta\varphi_x^{\tau} - \frac{1}{2}(1 + \eta)h^2\rho_x. \quad (2.74)$$

It can be shown that for the over-relaxation algorithm to converge, η is constrained by

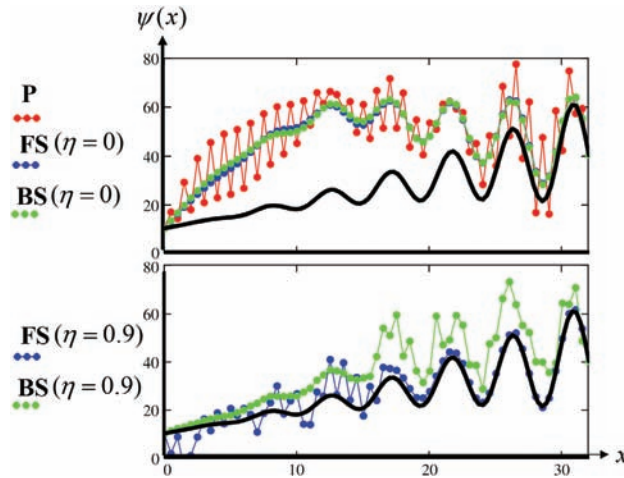


Figure 2.8 Top: Comparison of the parallel algorithm (P, red), the forward serial (FS, blue), and the backward serial (BS, green) algorithms with $\eta = 0$. Bottom: The FS and the BS algorithms with $\eta = 0.9$. Analytical solution is the solid black line in both top and bottom. 29 iterations.

$$0 \leq \eta < 1. \quad (2.75)$$

However, when η is too close to unity (e.g., $\eta = 0.99$), φ_χ^τ oscillates about the analytic solution with respect to both χ and τ . Although the oscillation decays with increasing τ , the closer η is to unity the slower this decay. Numerical experiments show that for $\eta = 0.90$, the oscillations quickly decay and give fast convergence to the analytic solution. Figure 2.8 illustrates the convergence behavior of the different relaxation algorithms and different relaxation parameters. (See Program MC2.2 for an implementation and comparison of different relaxation algorithms.)

2.8 The Random Walk Model and the Diffusion Equation

2.8.1 Random walk model

All of the algorithms introduced so far are deterministic algorithms, in which the output is completely determined by the input (at least in principle). There is another class of algorithms called “stochastic,” in which the output is statistically correlated with the input (but not independent of it).

The random walk model of Brownian motion has an illustrious history, and there is abundant literature on the subject—see, for example, Refs. 13 and 14. We briefly introduce it here as an example of a stochastic algorithm.

In a 2D random walk, a particle starts at time $t = 0$ at position $(0, 0)$ on a grid defined by $x = nh$ and $y = mh$, where $h = \Delta x = \Delta y$, and $n, m = 0, \pm 1, \pm 2, \dots$

Discretizing time by $t = \tau\Delta t$ with $\tau = 0, 1, 2, \dots$, let $\mathbf{x}_\tau = (x_\tau, y_\tau)$ be the position at $t = \tau\Delta t$. At $t + \Delta t$, the particle's position is

$$\mathbf{x}_{\tau+1} = \mathbf{x}_\tau + \Delta\mathbf{x}_\tau, \quad (2.76)$$

where $\Delta\mathbf{x}_\tau = (+h, 0), (-h, 0), (0, +h)$, and $(0, -h)$ with probability p_1, p_2, p_3, p_4 , respectively. For simplicity, we analyze the case where $p_1 = p_2 = p_3 = p_4 = 1/4$, which is the usual random walk model. Equation (2.76) is called a stochastic difference equation.

Now consider an infinite ensemble of identical particles. Since all of the probabilities are equal, the value of $\Delta\mathbf{x}_\tau$ averaged over all particles (the ensemble average, denoted by angle brackets) is

$$\langle \Delta\mathbf{x}_\tau \rangle = (0, 0). \quad (2.77)$$

Taking the ensemble average of Eq. (2.76), we find that

$$\langle \mathbf{x}_{\tau+1} \rangle = \langle \mathbf{x}_\tau + \Delta\mathbf{x}_\tau \rangle = \langle \mathbf{x}_\tau \rangle. \quad (2.78)$$

Thus, the ensemble average position is constant, regardless of its initial value.

Since the particles must move one space step in every time step, $\Delta\mathbf{x}_\tau \bullet \Delta\mathbf{x}_\tau = h^2$ and, hence, $\langle \Delta\mathbf{x}_\tau^2 \rangle = h^2$. Thus,

$$\begin{aligned} \langle \mathbf{x}_{\tau+1}^2 \rangle &= \langle \mathbf{x}_{\tau+1}^2 + 2\mathbf{x}_\tau \bullet \Delta\mathbf{x}_\tau + h^2 \rangle \\ &= \langle \mathbf{x}_\tau^2 \rangle + h^2 \end{aligned} \quad (2.79)$$

because $\langle \mathbf{x}_\tau \bullet \Delta\mathbf{x}_\tau \rangle = 0$. Iterating Eq. (2.79) from $\tau = 0$, we find that

$$\langle \mathbf{x}_\tau^2 \rangle = \tau h^2. \quad (2.80)$$

Although $\mathbf{x}_\tau$ is a stochastic quantity given by a stochastic algorithm, $\langle \mathbf{x}_\tau^2 \rangle$ is a deterministic quantity.

2.8.2 Diffusion equation

With reference to Fig. 2.9, let $n_{x,y}^\tau$ be the number of particles within a square of area h^2 centered on (x, y) at time $t = \tau\Delta t$ (in the model the particles are all initially located in the center). The particle density is thus $\rho(x, y, t) = n_{x,y}^\tau/h^2$. During time interval Δt , the number of particles that leave the square is $n_{x,y}^\tau$ (because all particles move at each time step), while the number of particles that enter the square from neighboring points is

$$\frac{1}{4}(n_{x+h,y}^\tau + n_{x-h,y}^\tau + n_{x,y+h}^\tau + n_{x,y-h}^\tau);$$

hence,

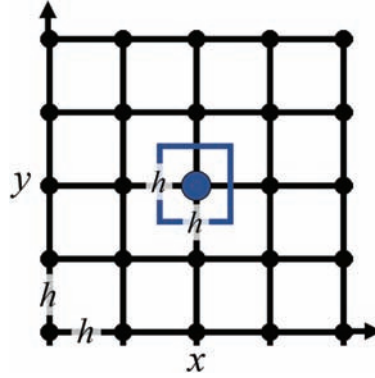


Figure 2.9 Particle distribution on a grid. Density is defined at each grid point.

$$n_{x,y}^{\tau+1} - n_{x,y}^{\tau} = \frac{1}{4}(n_{x+h,y}^{\tau} + n_{x-h,y}^{\tau} + n_{x,y+h}^{\tau} + n_{x,y-h}^{\tau} - 4n_{x,y}^{\tau}). \quad (2.81)$$

Dividing Eq. (2.81) by $\Delta t h^2$, and taking the limit $\Delta t \rightarrow 0$, $n_{x,y}^{\tau+1} - n_{x,y}^{\tau} = h^2 \Delta t \partial_t \rho(x,y,t)$, and we obtain

$$\begin{aligned} \partial_t \rho(x,y,t) = \frac{1}{4\Delta t} [\rho(x+h,y,t) + \rho(x-h,y,t) + \rho(x,y+h,t) \\ + \rho(x,y-h,t) - 4\rho(x,y,t)]. \end{aligned} \quad (2.82)$$

From Eqs. (1.25) and (1.26), we recognize the expression on the right to be $\mathbf{d}^2 \rho(\mathbf{x},t) \cong h^2 \nabla^2 \rho(\mathbf{x},t)$. In the limit $h \rightarrow 0$, Eq. (2.76) thus becomes

$$\partial_t \rho(x,y,t) = \mu \nabla^2 \rho(x,y,t), \quad (2.83)$$

where $\mu = h^2/4\Delta t$. This is the diffusion equation, and μ is the diffusion coefficient.

Using the random walk model, Albert Einstein (in 1905) and Marian Smoluchowski (in 1906) independently clarified the physical and mathematical basis of Brownian motion.

2.8.3 1D random walk

In one dimension, Eq. (2.82) reduces to $x_{\tau+1} = x_{\tau} + \Delta x_{\tau}$. Figure 2.10 shows a plot of x_{τ} for $\Delta x_{\tau} = \pm h$ with equal probability. It can be shown that the graph is a fractal in the limits $h, \Delta t \rightarrow 0$. In 1900, Louis Bachelier in his Ph.D. dissertation “The Theory of Speculation” showed that price movements on stock and option markets can be modeled as Brownian motion.

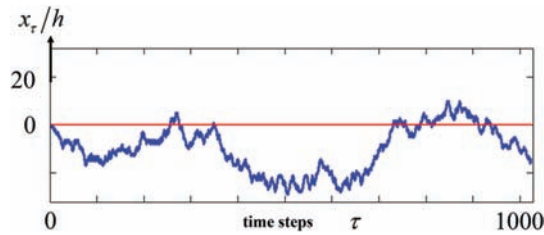


Figure 2.10 1D random walk with one particle.

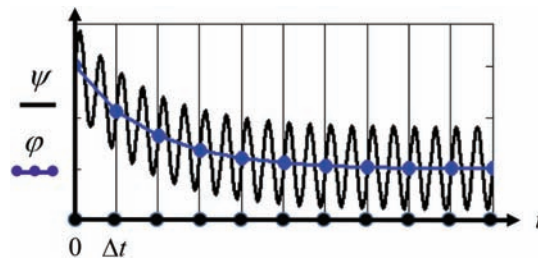


Figure 2.11 Although the numerical solution $\varphi(\tau\Delta t)$ matches the analytical solution $\psi(t)$, at $t = \tau\Delta t$, ψ and φ may be quite different.

Important Points of Chapter 2

- Differential equations can be solved by approximating them with difference equations, which can be solved numerically. Even when there is no numerical instability or chaos, the solution $\psi(t)$ of the differential equation can be very different from the solution $\varphi(t)$ of the corresponding difference equation, as shown in Fig. 2.11.
- The most accurate algorithm may be numerically unstable.
- Deterministic chaos afflicts many kinds of numerical algorithms.
- To avoid numerical instability, the order of the FD approximations in the FD model of a differential equation should match the order of the derivatives of the differential equation, but this alone does not guarantee stability, especially for nonlinear problems.
- Nonlocal models of nonlinear terms in a differential equation can avert numerical instability.
- Before constructing an algorithm and choosing its parameters, it is advisable to gain as much information as possible about the solutions sought, based on physical insight.
- Parallel algorithms do not necessarily converge faster than serial algorithms.

Appendix 2.1 Matrix Formulations of Relaxation

The relaxation algorithms can be expressed in matrix form. Although of little use for practical calculations, this formulation is useful to prove convergence

and yields some interesting insights. For simplicity, we do this in one dimension where ψ and ρ can be represented as a column matrices of $N+1$ rows:

$$\psi^T = [\psi_0 \quad \psi_1 \quad \cdots \quad \psi_{N-1} \quad \psi_N], \quad (\text{A2.1.1a})$$

$$\rho^T = [\rho_0 \quad \rho_1 \quad \cdots \quad \rho_{N-1} \quad \rho_N], \quad (\text{A2.1.1b})$$

where $\mathbf{M}^T$ is the transpose of $\mathbf{M}$.

A2.1.1 Parallel relaxation

Parallel relaxation computes

$$\begin{aligned} \varphi_{\chi}^{\tau+1} &= \frac{1}{2}(\varphi_{\chi-1}^{\tau} + \varphi_{\chi+1}^{\tau}) - \frac{1}{2}h^2\rho_{\chi} & \text{for } 1 \leq \chi \leq N-1, \\ \varphi_{\chi}^{\tau+1} &= \varphi_{\chi}^{\tau} & \text{for } \chi = 0, N. \end{aligned} \quad (\text{A2.1.2})$$

To cast this into matrix form, we seek matrices $\mathbf{R}_{\pm}$ such that $(\mathbf{R}_{\pm}\psi)_{\chi} = \psi_{\chi\pm 1}/2$ for $1 \leq \chi \leq N-1$, and $(\mathbf{R}_{\pm}\psi)_{\chi} = \psi_{\chi}/2$ for $\chi = 0, N$. We easily find that

$$\begin{aligned} \mathbf{R}_+ &= \frac{1}{2} \begin{bmatrix} 1 & 0 & \cdots & & 0 \\ 0 & 0 & 1 & 0 & \cdots & \vdots \\ & & 0 & 1 & 0 & \\ \vdots & \vdots & \vdots & \ddots & \ddots & \\ & & & & 0 & 1 \\ 0 & \cdots & & & 0 & 1 \end{bmatrix}, \\ \mathbf{R}_- &= \frac{1}{2} \begin{bmatrix} 1 & 0 & \cdots & & 0 \\ 1 & 0 & 0 & 0 & \cdots & \vdots \\ 0 & 1 & 0 & & 0 & \\ \vdots & \vdots & \ddots & \ddots & \ddots & \\ & & & 1 & 0 & 0 \\ 0 & \cdots & & & 0 & 1 \end{bmatrix}. \end{aligned} \quad (\text{A2.1.3})$$

We then define the parallel relaxation matrix by

$$\mathbf{R}_p = \mathbf{R}_+ + \mathbf{R}_-. \quad (\text{A2.1.4})$$

$\mathbf{J}$ is defined so that $(\mathbf{J}\rho)_{\chi} = \rho_{\chi}$ for $1 \leq \chi \leq N-1$, and $(\mathbf{J}\rho)_{\chi} = 0$ for $\chi = 0, N$. Thus, it leaves the interior elements of ρ unchanged and sets the boundary

elements to zero so that they do not affect the boundary values of ψ in the relaxation algorithm:

$$\mathbf{J} = \begin{bmatrix} 0 & 0 & \cdots & & & 0 \\ 0 & 1 & & 0 & 0 & \vdots \\ & & & 1 & 0 & \\ \vdots & \vdots & & \vdots & \ddots & \\ 0 & \cdots & & & 1 & 0 \\ & & & & 0 & 0 \end{bmatrix}. \quad (\text{A2.1.5})$$

The FD model of Poisson's equation in matrix form is thus

$$\psi = \mathbf{R}_p \psi - \frac{1}{2} h^2 \mathbf{J} \rho, \quad (\text{A2.1.6})$$

and the parallel relaxation algorithm becomes

$$\varphi^{\tau+1} = \mathbf{R}_p \varphi^\tau - \frac{1}{2} h^2 \mathbf{J} \rho. \quad (\text{A2.1.7})$$

Iterating Eq. (A2.1.7) from $\tau=0$, we find that

$$\varphi^\tau = \mathbf{R}_p^\tau \varphi^0 - \frac{1}{2} h^2 \mathbf{S}_p^\tau \rho, \quad (\text{A2.1.8})$$

where

$$\mathbf{S}_p^\tau = \sum_{m=0}^{\tau-1} \mathbf{R}_p^m \mathbf{J}. \quad (\text{A2.1.9})$$

A2.1.2 Serial relaxation

The forward serial relaxation algorithm given by Eq. (2.71) in matrix form is

$$\varphi^{\tau+1} = \mathbf{R}_- \varphi^{\tau+1} + \mathbf{R}_+ \varphi^\tau - \frac{1}{2} h^2 \mathbf{J} \rho. \quad (\text{A2.1.10})$$

Solving for $\varphi^{\tau+1}$, we find that

$$\begin{aligned} \varphi^{\tau+1} &= [\mathbf{1} - \mathbf{R}_-]^{-1} \mathbf{R}_+ \varphi^\tau - \frac{1}{2} h^2 [\mathbf{1} - \mathbf{R}_-]^{-1} \mathbf{J} \rho \\ &= \mathbf{R}_s \varphi^\tau - \frac{1}{2} h^2 [\mathbf{1} - \mathbf{R}_-]^{-1} \mathbf{J} \rho, \end{aligned} \quad (\text{A2.1.11})$$

where $\mathbf{1}$ is the unit matrix, and $\mathbf{R}_s = (\mathbf{1} - \mathbf{R}_-)^{-1} \mathbf{R}_+$ is the serial relaxation matrix. Evaluating $\mathbf{R}_s$, we find that

$$\mathbf{R}_s = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 2^{-1} & 0 & 2^{-1} & 0 & 0 & 0 \\ \vdots & 0 & \vdots & 2^{-1} & 0 & 0 \\ 2^{-(N-2)} & 0 & 2^{-(N-2)} & \vdots & 2^{-1} & 0 \\ 2^{-(N-1)} & 0 & 2^{-(N-1)} & 2^{-(N-2)} & \dots & 2^{-1} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \quad (\text{A2.1.12})$$

Iterating Eq. (A2.1.11) from $\tau=0$, we obtain

$$\varphi^\tau = \mathbf{R}_s^\tau \varphi^0 - \frac{1}{2} h^2 \mathbf{S}_s^\tau \rho, \quad (\text{A2.1.13})$$

where

$$\mathbf{S}_s^\tau = \sum_{m=0}^{\tau-1} \mathbf{R}_s^m (\mathbf{1} - \mathbf{R}_s)^{-1} \mathbf{J}. \quad (\text{A2.1.14})$$

A2.1.3 Over-relaxation

The forward serial over-relaxation algorithm [Eq. (2.74), repeated below]

$$\varphi_{\chi}^{\tau+1} = \frac{1}{2} (1 + \eta) \left(\varphi_{\chi-1}^{\tau+1} + \varphi_{\chi+1}^{\tau} \right) - \eta \varphi_{\chi}^{\tau} - \frac{1}{2} (1 + \eta) h^2 \rho_{\chi} \quad (\text{A2.1.15})$$

can be expressed in matrix form as

$$\varphi^{\tau+1} = (1 + \eta) \mathbf{R}_- \varphi^{\tau+1} + [(1 + \eta) \mathbf{R}_+ - \eta \mathbf{1}] \varphi^{\tau} - \frac{1}{2} h^2 \mathbf{J} \rho. \quad (\text{A2.1.16})$$

Solving for $\varphi^{\tau+1}$, we obtain

$$\begin{aligned} \varphi^{\tau+1} &= [\mathbf{1} - (1 + \eta) \mathbf{R}_-]^{-1} [(1 + \eta) \mathbf{R}_+ - \eta \mathbf{1}] \varphi^{\tau} - \frac{1}{2} h^2 [\mathbf{1} - (1 + \eta) \mathbf{R}_-]^{-1} \mathbf{J} \rho \\ &= \mathbf{R}_o(\eta) \varphi^{\tau} - \frac{1}{2} h^2 [\mathbf{1} - (1 + \eta) \mathbf{R}_-]^{-1} \mathbf{J} \rho, \end{aligned} \quad (\text{A2.1.17})$$

where $\mathbf{R}_o(\eta) = [\mathbf{1} - (1 + \eta) \mathbf{R}_-]^{-1} [(1 + \eta) \mathbf{R}_+ - \eta \mathbf{1}]$ is the forward serial over-relaxation matrix.

Note A2.1.1

From Eq. (A2.1.11), one might define

$$\Delta \varphi^{\tau} = (\mathbf{R}_s - \mathbf{1}) \varphi^{\tau} - \frac{1}{2} h^2 (\mathbf{1} - \mathbf{R}_s)^{-1} \mathbf{J} \rho, \quad (\text{A2.1.18})$$

and then with the substitution $\Delta \varphi_{\tau} \rightarrow (1 + \eta) \Delta \varphi_{\tau}$ obtain

$$\varphi^{\tau+1} = [(1 + \eta)\mathbf{R}_s - \eta\mathbf{1}]\varphi^\tau - \frac{1}{2}(1 + \eta)h^2(\mathbf{1} - \mathbf{R}_-)^{-1}\mathbf{J}\rho, \quad (\text{A2.1.19})$$

but this is not what Program PC2.3 computes.

Iterating Eq. (A2.1.17) from $\tau=0$, we find that

$$\varphi^\tau = \mathbf{R}_o^\tau(\eta)\varphi^0 - \frac{1}{2}h^2\mathbf{S}_o^\tau(\eta)\rho, \quad (\text{A2.1.20})$$

where

$$\mathbf{S}_o^\tau(\eta) = (1 + \eta) \sum_{m=0}^{\tau-1} \mathbf{R}_o^m(\eta) [\mathbf{1} - (1 + \eta)\mathbf{R}_-]^{-1}\mathbf{J}. \quad (\text{A2.1.21})$$

A2.1.4 Convergence

Let us now examine the limit of an infinite number of iterations. Defining $\mathbf{R}^\infty = \lim_{\tau \rightarrow \infty} \mathbf{R}^\tau$, where $\mathbf{R} = \mathbf{R}_p$, $\mathbf{R}_s$, or $\mathbf{R}_o$, $\mathbf{R}^\infty$ can be determined from the requirement that $\mathbf{R}\mathbf{R}^\infty = \mathbf{R}^\infty\mathbf{R} = \mathbf{R}^\infty$. We find that all of the limits are the same. Denoting this limit by $\mathbf{R}^\infty$, $\mathbf{R}_p^\infty = \mathbf{R}_s^\infty = \mathbf{R}_o^\infty(\eta) = \mathbf{R}^\infty$, where

$$\mathbf{R}^\infty = \frac{1}{N} \begin{bmatrix} N & 0 & 0 & \cdots & 0 & 0 \\ N-1 & \vdots & \vdots & \vdots & \vdots & 1 \\ \vdots & & & & & \\ & & & & \vdots & \\ 1 & & & & & N-1 \\ 0 & 0 & 0 & \cdots & 0 & N \end{bmatrix}. \quad (\text{A2.1.22})$$

Evaluating $\varphi_L^\infty = \mathbf{R}^\infty \varphi^0$, we find that

$$\varphi_{L,x}^\infty = \psi_0 + \frac{\chi}{N}(\psi_N - \psi_0). \quad (\text{A2.1.23})$$

For all φ^0 that have the same boundary values as ψ ($\varphi_0^0 = \psi_0$ and $\varphi_N^0 = \psi_N$), φ_L^∞ is equivalent to the analytical solution [Eq. (2.69)] of the Laplace equation for the case where $\rho=0$.

Next, we evaluate the sums $\mathbf{S}_p^\tau$, $\mathbf{S}_s^\tau$, and $\mathbf{S}_o^\tau(\eta)$, given by Eqs. (A2.1.9), (A2.1.14), and (A2.1.21), respectively. $\mathbf{S}_p^\tau = \sum_{m=0}^{\tau-1} \mathbf{R}_p^m \neq [\mathbf{1} - \mathbf{R}_p]^{-1}[\mathbf{1} - \mathbf{R}_p^\tau]$ because the inverse $[\mathbf{1} - \mathbf{R}_p]^{-1}$ does not exist. However, using the fact that

$$\mathbf{R}_p\mathbf{J} = \mathbf{J}\mathbf{R}_p\mathbf{J} \quad (\text{A2.1.24})$$

for $\mathbf{R} = \mathbf{R}_p$, $\mathbf{R}_s$, and $\mathbf{R}_o$, it is then easy to show that

$$\mathbf{R}_p^\tau \mathbf{J} = (\mathbf{R}_p \mathbf{J})^\tau \quad (\text{A2.1.25})$$

for $\tau \geq 1$. Hence, $\mathbf{S}_p^\tau = \mathbf{S}_p'^\tau \mathbf{J}$ is given by

$$\begin{aligned} \mathbf{S}_p^\tau &= \left[\sum_{m=0}^{\tau-1} (\mathbf{R}_p \mathbf{J})^m \right] \mathbf{J} \\ &= (\mathbf{1} - \mathbf{R}_p \mathbf{J})^{-1} \left[\mathbf{1} - (\mathbf{R}_p \mathbf{J})^\tau \right] \mathbf{J} \end{aligned} \quad (\text{A2.1.26})$$

because $(\mathbf{1} - \mathbf{R}\mathbf{J})^{-1}$ does exist for $\mathbf{R} = \mathbf{R}_p$, $\mathbf{R}_s$, and $\mathbf{R}_o$; furthermore,

$$\lim_{\tau \rightarrow \infty} (\mathbf{R}\mathbf{J})^\tau = 0. \quad (\text{A2.1.27})$$

Thus,

$$\mathbf{S}_p^\infty = (\mathbf{1} - \mathbf{R}_p \mathbf{J})^{-1} \mathbf{J}. \quad (\text{A2.1.28})$$

Note A2.1.2

From Eq. (A2.1.22), $\mathbf{R}^\infty \boldsymbol{\varphi} = \mathbf{0}$ (here $\mathbf{0}$ is a column matrix with all elements equal to zero) for any column vector $\boldsymbol{\varphi}$ for which the boundary elements are zero, i.e., $\varphi_0 = \varphi_N = 0$. Since the first and last elements of all of the columns of $\mathbf{J}$ are zero, $\mathbf{R}^\infty \mathbf{J} = \mathbf{0}$. Equation (A2.1.27) then follows from Eq. (A2.1.25).

To evaluate $\mathbf{S}_s^\tau$, we again use Eq. (A2.1.25) together with the fact that

$$(\mathbf{1} - \mathbf{R}_-)^{-1} \mathbf{J} = \mathbf{J}(\mathbf{1} - \mathbf{R}_-)^{-1} \mathbf{J} \quad (\text{A2.1.29})$$

and find that

$$\mathbf{S}_s^\tau = (\mathbf{1} - \mathbf{R}_s \mathbf{J})^{-1} [\mathbf{1} - (\mathbf{R}_s \mathbf{J})^\tau] (\mathbf{1} - \mathbf{R}_-)^{-1} \mathbf{J}, \quad (\text{A2.1.30})$$

and hence,

$$\mathbf{S}_s^\infty = (\mathbf{1} - \mathbf{R}_s \mathbf{J})^{-1} (\mathbf{1} - \mathbf{R}_-)^{-1} \mathbf{J}. \quad (\text{A2.1.31})$$

Finally, to evaluate $\mathbf{S}_o^\tau(\eta)$, we use the fact that

$$[\mathbf{1} - (1 + \eta)\mathbf{R}_-]^{-1} \mathbf{J} = \mathbf{J}[\mathbf{1} - (1 + \eta)\mathbf{R}_-]^{-1} \mathbf{J} \quad (\text{A2.1.32})$$

to obtain

$$\mathbf{S}_o^\tau(\eta) = (1 + \eta) [\mathbf{1} - \mathbf{R}_o(\eta)\mathbf{J}]^{-1} [\mathbf{1} - (\mathbf{R}_o(\eta)\mathbf{J})^\tau] [\mathbf{1} - (1 + \eta)\mathbf{R}_-]^{-1} \mathbf{J}, \quad (\text{A2.1.33})$$

and

$$\mathbf{S}_o^\infty(\eta) = (1 + \eta)[1 - \mathbf{R}_o(\eta)\mathbf{J}]^{-1}[1 - (1 + \eta)\mathbf{R}_-]^{-1}\mathbf{J}. \quad (\text{A2.1.34})$$

Furthermore, if the parallel, serial, and over-relaxed algorithms all converge to the same result, we expect that $\mathbf{S}_p^\infty = \mathbf{S}_s^\infty = \mathbf{S}_o^\infty(\eta) \equiv \mathbf{S}^\infty$. This turns out to be the case, and it can be shown that $\mathbf{S}^\infty$ is given by

$$\begin{aligned} \mathbf{S}_{i,j}^\infty &= 2(N-i)j && \text{for } i = 0, 1, \dots, N \\ &&& \text{and } j = 0, 1, \dots, i \\ \mathbf{S}_{i,j}^\infty &= \mathbf{S}_{j,i}^\infty && \text{otherwise,} \end{aligned} \quad (\text{A2.1.35})$$

where the rows and columns are numbered from 0 to N . The relaxation solution to Poisson's equation is thus

$$\varphi^\infty = \mathbf{R}^\infty \varphi^0 - \frac{1}{2} h^2 \mathbf{S}^\infty \rho \quad (\text{A2.1.36})$$

and is exactly equivalent to the analytic solution given by Eq. (2.69).

A2.1.5 Two dimensions

In two dimensions, let $(x, y) = (i, j)h$, where $h = \Delta x = \Delta y$, and let the solution domain be $(0 \leq x \leq N_x h) \times (0 \leq y \leq N_y h)$. Defining $\psi_{i,j} = \psi(ih, jh)$, ψ and φ^T can be represented as $(N_x+1) \times (N_y+1)$ matrices:

$$\psi = \begin{pmatrix} \psi_{0,0} & \psi_{0,1} & \cdots & \psi_{0,N_x-1} & \psi_{0,N_x} \\ \psi_{1,0} & & & & \psi_{1,N_x} \\ \vdots & & & & \vdots \\ \psi_{N_y-1,0} & & & & \psi_{N_y-1,N_x} \\ \psi_{N_y,0} & \psi_{N_y,1} & \cdots & \psi_{N_y,N_x-1} & \psi_{N_y,N_x} \end{pmatrix}. \quad (\text{A2.1.37})$$

If the outer rows and columns of matrix Eq. (A2.1.37) represent the boundary of the problem domain, then the initial guess solution is

$$\varphi^0 = \begin{pmatrix} \psi_{0,0} & \psi_{0,1} & \cdots & \psi_{0,n_x-1} & \psi_{0,n_x} \\ \psi_{1,0} & & & & \psi_{1,n_x} \\ \vdots & & \text{guess} & & \vdots \\ \psi_{n_y-1,0} & & \text{values} & & \psi_{n_y-1,n_x} \\ \psi_{n_y,0} & \psi_{n_y,1} & \cdots & \psi_{n_y,n_x-1} & \psi_{n_y,n_x} \end{pmatrix}. \quad (\text{A2.1.38})$$

It is easy to see that

$$(\mathbf{R}_p \psi)_{i,j} = \frac{\psi_{i+1,j} + \psi_{i-1,j}}{2}; \quad (\text{A2.1.39})$$

thus,

$$\frac{\psi_{i,j+1} + \psi_{i,j-1}}{2} = (\mathbf{R}_p \boldsymbol{\varphi}^T)_{i,j}^T = (\boldsymbol{\varphi} \mathbf{R}_p^T)_{i,j}. \quad (\text{A2.1.40})$$

Hence,

$$(\mathbf{R}_p + \boldsymbol{\varphi} \mathbf{R}_p^T)_{i,j} = \frac{\psi_{i,j+1} + \psi_{i,j-1} + \psi_{i+1,j} + \psi_{i-1,j}}{4}. \quad (\text{A2.1.41})$$

However, $\mathbf{R}_p$ acts on boundaries $\psi_{1,0}$ and $\psi_{i,N}$, while $\mathbf{R}_p^T$ acts on boundaries $\psi_{N,j}$ and $\psi_{0,j}$. To restore the boundary conditions on ψ , we set the boundary elements of $\mathbf{R}_p \psi + \psi \mathbf{R}_p^T$ to 0 by multiplying on the left and right by $\mathbf{J}$ and adding $\mathbf{B} = \psi - \mathbf{J} \psi \mathbf{J}$, which is a matrix with zeros in the interior but with the boundary values of φ . We can now express 2D relaxation in the form

$$\psi = \frac{1}{2} \mathbf{J} (\mathbf{R}_p \psi + \psi \mathbf{R}_p^T) \mathbf{J} + \mathbf{B}. \quad (\text{A2.1.42})$$

Obviously, matrix formulations of the relaxation algorithm in more than one dimension are quite complicated and so will not be further discussed.

Appendix 2.2 Noninteger-Order Integrals and Derivatives

Although not relevant to the main subject of this book, noninteger-order derivatives and integrals are useful in a variety of fields, including electromagnetism. This material in this appendix complements Appendix 1.2.

A2.2.1 Noninteger-order integration

We define the integration operator I acting on a function f by

$$If|_0^x = \int_0^x dt f(t). \quad (\text{A2.2.1})$$

The lower integration limit in this definition is arbitrary and can be chosen to suit the particular problem of interest. Iterating the integration,

$$I^2 f|_0^x = \int_0^x dt \int_0^t dt' f(t'). \quad (\text{A2.2.2})$$

To integrate by parts, let $F(t) = \int_0^t dt' f(t')$ so that by definition $\partial_t F(t) = f(t)$ and $I^2 f|_0^x = \int_0^x dt F(t)$. Using $\int_0^x dt \partial_t [t F(t)] = x F(x) = x \int_0^x dt f(t)$, we obtain

$$I^2 f|_0^x = \int_0^x dt (x - t) f(t). \quad (\text{A2.2.3})$$

By induction, it can be shown that

$$I^n f|_0^x = \frac{1}{(n-1)!} \int_0^x dt (x-t)^{n-1} f(t) \quad (\text{A2.2.4a})$$

$$= \frac{1}{\Gamma(n)} \int_0^x dt (x-t)^{n-1} f(t). \quad (\text{A2.2.4b})$$

[See Note A1.2.1. Since Γ is defined for noninteger arguments, Eq. (A2.2.4b) holds even when $n \geq 0$ is not an integer.]

Let us now evaluate the limit $n \rightarrow 0$. Integrating Eq. (A2.2.4b) by parts, we find that

$$\frac{1}{\Gamma(n)} \int_0^x dt (x-t)^{n-1} f(t) = \frac{1}{\Gamma(n)} \left[\frac{x^n}{n} f(0) + \frac{1}{n} \int_0^x dt (x-t)^n f'(t) \right]. \quad (\text{A2.2.5})$$

Using $\lim_{x \rightarrow 0} 1/\Gamma(x) = 0$ from Eq. (A1.2.16), we find that

$$\lim_{n \rightarrow 0} I^n f|_0^x = f(x); \quad (\text{A2.2.6})$$

hence,

$$I^0 = \mathbf{1}, \quad (\text{A2.2.7})$$

where $\mathbf{1}$ is the identity operator.

Example 1

Let $f(x) = x$ and evaluate the n -fold integral. Using Eq. (A2.2.4b), we find that

$$I^n f|_0^x = \frac{1}{\Gamma(n)} \int_0^x dt t (x-t)^{n-1} = \frac{x^{n+1}}{\Gamma(n+2)}. \quad (\text{A2.2.8})$$

Thus, $I^1 x|_0^x = x^2/2$, as expected. Using $\Gamma(n+1) = n\Gamma(n)$, and $\Gamma(1/2) = \sqrt{\pi}$, we find that $I^{1/2} f|_0^x = 4x^{3/2}/3\sqrt{\pi}$.

A2.2.2 Noninteger-order differentiation

We define the derivative operator ∂ and its n -fold action on a function f by

$$\partial^n f(x) = \frac{d^n}{dx^n} f(x) \quad (\text{A2.2.9})$$

for integer $n > 0$. It is easy to show that

$$\partial I f|_0^x = f(x), \quad (\text{A2.2.10})$$

and hence

$$\partial I = \mathbf{1}. \quad (\text{A2.2.11})$$

∂ is thus the left inverse of I , $\partial = I^{-1}$, and furthermore, for integer $n \geq 0$, it is easy to see that

$$\partial^n = I^{-n}. \quad (\text{A2.2.12})$$

On the other hand,

$$I \partial \neq \mathbf{1} \quad (\text{A2.2.13})$$

because

$$\begin{aligned} I \partial f|_0^x &= \int_0^x dt f(t) \\ &= f(x) - f(0). \end{aligned} \quad (\text{A2.2.14})$$

Using $\partial^n = I^{-1}$ in Eq. (A2.2.4b), one might try to extend the definition derivative to a noninteger $n \geq 0$, but since differentiation and integration do not commute, it is best to extend the definition of the derivative using conventional derivatives as far as possible. Let $0 \leq \nu \leq 1$, then

$$\partial^\nu = \partial \partial^{\nu-1} = \partial \partial^{-(1-\nu)} = \partial I^{1-\nu}; \quad (\text{A2.2.15})$$

hence, using Eq. (A2.2.4b),

$$\partial^\nu f(x) = \frac{1}{\Gamma(1-\nu)} \partial \int_0^x dt \frac{f(t)}{(x-t)^\nu}. \quad (\text{A2.2.16})$$

Setting $\nu=0$ in Eq. (A2.16), we obtain $\partial^0 f(x) = f(x)$; thus,

$$\partial^0 = \mathbf{1}. \quad (\text{A2.2.17})$$

Integrating by parts in Eq. (A2.2.16), we find that

$$\lim_{\nu \rightarrow 1} \frac{1}{\Gamma(1-\nu)} \int_0^x dt \frac{f(t)}{(x-t)^\nu} = f(x), \quad (\text{A2.2.18})$$

so $\lim_{\nu \rightarrow 1} \partial^\nu = \partial$, as expected.

Using the identities

$$\frac{\partial}{\partial x} \int_0^x dt g(x, t) = g(x, t)|_{t=x} + \int_0^x dt \partial_x g(x, t) \quad (\text{A2.2.19})$$

and $\Gamma(x+1) = x\Gamma(x)$ in Eq. (A2.2.16), and setting $g(x, t) = f(t)/(x-t)^\nu$, we obtain

$$\begin{aligned} \frac{1}{\Gamma(1-\nu)} \partial \int_0^x dt \frac{f(t)}{(x-t)^\nu} &= \frac{1}{\Gamma(-\nu)} \int_0^x dt \frac{f(t)}{(x-t)^{\nu+1}} \\ &= I^{-\nu}[f](x). \end{aligned} \quad (\text{A2.2.20})$$

Thus, $\partial^\nu = I^{-\nu}$ for $0 \leq \nu \leq 1$, as expected.

Writing $\partial^{n+\nu} = \partial^\nu \partial^n$, where $n \geq 0$ is an integer, and $0 < \nu < 1$ is real, we can now compute $\partial^{n+\nu} f(x)$ in a two-step process:

$$g(x) = \frac{d^n}{dx^n} f(x), \quad (\text{A2.2.21a})$$

$$\partial^{n+\nu} f(x) = \partial^\nu g(x), \quad (\text{A2.2.21b})$$

where $\partial^\nu g(x)$ is computed using Eq. (A2.2.16).

While the integer-order derivative depends only on the values of f in an infinitesimal neighborhood about x , the noninteger-order derivative depends on the integration range in Eq. (A2.2.16). This integration range can be chosen to suit the application of interest.

Example 2

Evaluate $\partial^n x^2$ -fold for $0 < n < 1$. Using Eq. (A2.2.17), we find that

$$\partial^n x^2 = \frac{1}{\Gamma(1-n)} \partial_x \int_0^x dt \frac{t^2}{(x-t)^n} = \frac{2x^{2-n}}{\Gamma(1-n)(1-n)(2-n)}. \quad (\text{A2.2.22})$$

Putting $n=1$ into Eq. (A2.2.10), we find that $\partial(x^2) = 2x$, and $\partial^{1/2}(x^2) = 8x^{3/2}/3\sqrt{\pi}$.

Example 3

For simple power functions, the formula $\partial_x^n x^m = x^{m-n} m!/(m-n)!$ can be generalized to

$$\partial_x^n x^m = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} x^{m-n}, \quad (\text{A2.2.23})$$

which is valid for noninteger $n \leq m$ and m . In this case, noninteger-order derivatives depend only on the local value of x .

Further details on noninteger-order integration and differentiation can be found in Ref. 15. An interesting application of fractional derivatives to electromagnetism can be found in Refs. 16 and 17.

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Chapter 3

Finite Difference Models of the Simple Harmonic Oscillator

The simple harmonic oscillator (SHO) is the basis of many physical models. Since it can be solved analytically, it is a useful vehicle to introduce the basic concepts of the FDTD methodology without being distracted by the technical details needed to implement FDTD for the wave equation and for Maxwell's equations.

In this chapter we derive exact FDTD algorithms from *nonstandard* FD models to solve the free, damped, and damped and driven SHO. The concepts developed in this chapter will be subsequently extended to develop nonstandard, high-precision versions of FDTD to solve the wave equation and Maxwell's equations, which is one of the main purposes of this book.

We first develop analytical solutions against which numerical solutions can be compared.

Topics:

- FDTD algorithms
- Second-order versus fourth-order models
- Nonstandard finite difference models
- Numerical stability
- Discrete Green's function

3.1 Analytic Solution of the Simple Harmonic Oscillator

The SHO is described by

$$(\partial_t^2 + \omega^2)\psi(t) = 0, \quad (3.1)$$

where $\omega = 2\pi/T$ is the angular frequency, and T is the oscillation period. General solutions are

$$\begin{aligned}\psi(t) &= a_+ e^{i\omega t} + a_- e^{-i\omega t} \\ &= a_s \sin(\omega t) + a_c \cos(\omega t),\end{aligned}\quad (3.2)$$

where the constants $a_{\pm}$ (or $a_{s,c}$) are determined by the two initial conditions

$$\psi(0) = \psi_0, \quad (3.3a)$$

$$\psi'(0) = \psi'_0. \quad (3.3b)$$

These initial conditions model the release of a simple pendulum with angular velocity ψ'_0 at a distance ψ_0 from its equilibrium position, $\psi = 0$. For example if $\psi'_0 = 0$, the solution of Eq. (3.1) is

$$\psi(t) = \psi_0 \cos(\omega t). \quad (3.4)$$

3.2 Second-Order Finite Difference Model of the Simple Harmonic Oscillator

Approximating the derivative in Eq. (3.1) using the second-order central finite difference (CFD) expression [Eq. (1.10)], we obtain a (we use the indefinite article ‘a’ to emphasize that there can more than one) second-order FD model of the SHO,

$$(d_t^2 + \omega^2 \Delta t^2) \psi(t) = 0, \quad (3.5)$$

which we call the standard (S) FD model to distinguish it from the non-standard model (introduced later). From now on, unless otherwise specified, we put $d_t^c \rightarrow d_t$ and d_t^2 in place of $(d_t^c)^2$. From Eq. (A1.1.11), we see that this difference equation is equivalent to the differential equation

$$\left(\partial_t^2 + \omega^2 + \frac{1}{12} \Delta t^2 \partial_t^4 + \cdots \right) \psi(t) = 0. \quad (3.6)$$

We should not, therefore, be surprised to find that the solution of the difference equation [Eq. (3.5)] differs from that of the SHO.

Setting $t = \tau \Delta t$ ($\tau = 0, 1, 2, \dots$), $\psi_\tau = \psi(\tau \Delta t)$, and defining $d_\tau^2 \psi_\tau = \psi_{\tau+1} + \psi_{\tau-1} - 2\psi_\tau$, the S-FD model [Eq. (3.5)] of the SHO takes the form

$$(d_\tau^2 + \omega^2 \Delta t^2) \psi_\tau = 0. \quad (3.7)$$

Expanding $d_\tau^2 \psi_\tau$, Eq. (3.7) becomes

$$\psi_{\tau+1} + \psi_{\tau-1} - (2 - \omega^2 \Delta t^2) \psi_\tau = 0. \quad (3.8)$$

Equation (3.8) is a difference equation, which can be solved using the FDTD algorithm (in this simple case it can also be solved analytically).

Solving for $\psi_{\tau+1}$, we obtain what we call the S-FDTD algorithm,

$$\psi_{\tau+1} = -\psi_{\tau-1} + (2 - \omega^2 \Delta t^2) \psi_{\tau}. \quad (3.9)$$

Two initial conditions, ψ_0 and ψ_1 , determine ψ at all times $t > \Delta t$. Taking

$$\psi_0 = \psi(0), \quad (3.10a)$$

$$\psi_1 = \psi_0 \cos(\omega \Delta t), \quad (3.10b)$$

the S-FDTD algorithm [Eq. (3.9)] can be iterated and directly compared with the analytic solution.

Note 3.1

If we only knew ψ'_0 (but not ψ_1), we could use the estimate, $\psi_1 = \psi_0 + \psi'_0 \Delta t$.

The difference equation [Eq. (3.8)] can also be solved analytically. As shown in Appendix 3.1,

$$\psi_{\tau} = \psi_0 \left[\cos(\omega' \tau \Delta t) + \frac{\cos(\omega \Delta t) - \cos(\omega' \Delta t)}{\sin(\omega' \Delta t)} \sin(\omega' \tau \Delta t) \right], \quad (3.11)$$

where

$$\omega' \Delta t = 2 \arcsin(\omega \Delta t / 2). \quad (3.12)$$

It is shown in Appendix 3.2 that the S-FDTD algorithm is numerically stable if

$$-2 \leq \omega \Delta t \leq 2, \quad (3.13a)$$

or

$$\frac{T}{\Delta t} \geq \pi. \quad (3.13b)$$

3.3 Fourth-Order Finite Difference Model of the Simple Harmonic Oscillator

One might suppose that the accuracy of the FD model could be improved by substituting a fourth-order FD approximation to the second derivative in place of the second-order FD approximation. Using Eq. (1.15), we obtain

$$\left(d_t^2 - \frac{1}{12}d_t^4 + \omega^2\Delta t^2\right)\psi(t) = 0. \quad (3.14)$$

From Appendix 1.1, we see that this is equivalent to the differential equation,

$$\left(\partial_t^2 + \omega^2 - \frac{1}{90}\Delta t^4 \partial_t^6 - \frac{1}{1008}\Delta t^6 \partial_t^8 - \dots\right)\psi(t) = 0. \quad (3.15)$$

Comparing Eq. (3.6) with Eq. (3.15), we might conclude that Eq. (3.14) is a much better model of the SHO [Eq. (3.1)].

Expanding the FD operators in Eq. (3.14) (see Note A1.2.2), we obtain

$$-(\psi_{\tau+2} + \psi_{\tau-2}) + 16(\psi_{\tau+1} + \psi_{\tau-1}) - (30 - 12\omega^2\Delta t^2)\psi_{\tau} = 0; \quad (3.16)$$

hence, the fourth-order FDTD algorithm is

$$\psi_{\tau+1} = -\psi_{\tau-3} + 16(\psi_{\tau} + \psi_{\tau-2}) - (30 - 12\omega^2\Delta t^2)\psi_{\tau-1}. \quad (3.17)$$

Note 3.2

Four initial conditions are needed to iterate Eq. (3.17) instead of the two needed to solve the original differential equation. As we previously remarked, this is “unnatural” and can cause numerical instability.

Inserting the analytic solution $\varphi_0 = e^{i\omega t}$ into the second-order [Eq. (3.5)] and fourth-order [Eq. (3.14)] FD models, respectively, with $\omega\Delta t = 2\pi\Delta t/T = 2\pi/8$, we find that

$$\frac{1}{\varphi_0}(d_t^2 + \omega^2\Delta t^2)\varphi_0 = 0.031, \quad (3.18a)$$

$$\frac{1}{\varphi_0}\left(d_t^2 - \frac{1}{12}d_t^4 + \omega^2\Delta t^2\right)\varphi_0 = 0.0025. \quad (3.18b)$$

The deviations of the right sides of Eq. (3.18) from 0 measure the errors of the second- and fourth-order FD models, respectively. Since the error of the latter is an order of magnitude less than that of the former, one might presume the fourth-order FDTD algorithm to be more accurate than the second-order one.

However, these two models are fundamentally different (see Note 2.2). While both the second-order FDTD algorithm and the original differential equation require two initial conditions to specify a solution, the fourth-order FDTD one requires four. Analogously, $d^2\varphi(t)/dt^2 = 0$ and $d^4\varphi(t)/dt^4 = 0$ share a subset of solutions, but the latter has additional solutions that are very different from those of the former. In Appendix 3.2 we show that the

fourth-order FDTD algorithm is numerically unstable. Numerical experiments show that instability quickly sets in after just a few time steps.

As shown Appendix 3.2, the analytic solution of Eq. (3.16) is

$$\psi_\tau = a_{1+}e^{i\omega'\tau\Delta t} + a_{1-}e^{-i\omega'\tau\Delta t} + a_{2+}\lambda_{2+}^\tau + a_{2-}\lambda_{2-}^\tau, \quad (3.19)$$

where

$$\omega'\Delta t = \pm 2 \arcsin \left[\sqrt{\frac{3}{2}} \left(\sqrt{1 + \omega^2\Delta t^2/3} - 1 \right)^{1/2} \right], \quad (3.20)$$

and

$$\lambda_{2\pm} = 4 + \sqrt{3\omega^2\Delta t^2 + 9} \pm \sqrt{8\sqrt{3\omega^2\Delta t^2 + 9} + (3\omega^2\Delta t^2 + 24)}. \quad (3.21)$$

Because $\lambda_{2+} > 1$ for all values of $\omega\Delta t$, the fourth-order FDTD algorithm is unconditionally unstable.

In Fig. 3.1 we compare the second-order S-FDTD and the fourth-order FDTD (FDTD-4) solution with the analytic solution $\psi(t) = \cos(\omega t)$.

The phase error of the S-FDTD calculation increases with time but is numerically stable. In principle, the FDTD-4 calculation ought to be much more accurate than S-FDTD, but it is numerically unstable, and diverges after just a few time steps, as seen in Fig. 3.1.

3.4 Nonstandard Finite Difference Model of the Simple Harmonic Oscillator

We have seen that accuracy cannot be improved by using higher than second-order FD approximations because of numerical instability. However, using only second-order FD expressions in a nonstandard model, it is possible to construct an exact model of the SHO.

Replacing $\omega\Delta t$ with $\tilde{\omega}$ in the second-order model [Eq. (3.5)], and regarding $\tilde{\omega}$ as a free parameter, we seek $\tilde{\omega}$ such that the solution of the FD model

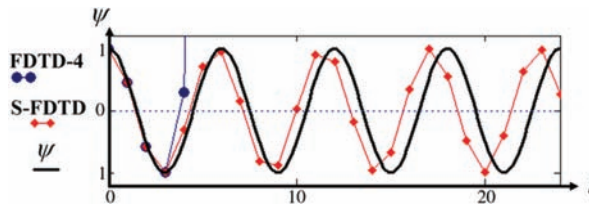


Figure 3.1 Analytic solution ψ versus numerical solution. S-FDTD is the conventional second-order FDTD [Eq. (3.9)], and FDTD-4 is the fourth-order FDTD [Eq. (3.17)]; $T = \text{oscillator period} = 6\Delta t$.

$$(d_t^2 + \tilde{\omega}^2)\psi(t) = 0 \quad (3.22)$$

is the same as the solution of the SHO. Taking $\psi(t) = e^{i\omega t}$, we find that

$$(d_t^2 + \tilde{\omega}^2)e^{i\omega t} = 0 \quad (3.23)$$

if

$$\tilde{\omega} = 2 \sin(\omega \Delta t/2). \quad (3.24)$$

Equation (3.22) together with Eq. (3.24) is an example of a nonstandard (NS) FD model.¹ It is exact because the harmonic oscillator solutions and difference equation solutions are identical. An exact FDTD algorithm to solve the SHO equation is thus

$$\psi_{\tau+1} = -\psi_{\tau-1} + (2 - \tilde{\omega}^2)\psi_{\tau}. \quad (3.25)$$

This is an example of a NS-FDTD algorithm. In Fig. 3.2 we compare S- and NS-FDTD calculations with the analytic solution.

Using the methods of Appendix 3.1, we find that the NS-FDTD algorithm is numerically stable if

$$0 < \tilde{\omega} \leq 2. \quad (3.26)$$

Inserting Eq. (3.24) into Eq. (3.26) then gives $\sin(\omega\Delta t/2) \leq \sin(\pi/2)$, or

$$-\pi < \omega \Delta t < \pi, \quad (3.27a)$$

$$\frac{T}{\Delta t} > 2. \quad (3.27b)$$

Comparing this stability condition with Eq. (3.13), we see that a larger time step can be used in NS-FDTD. The condition given by Eq. (3.27b) is the maximum time step allowed by the Nyquist sampling theorem,¹ which states that a harmonic signal cannot be unambiguously reconstructed unless the sampling frequency is greater than $2/T$.

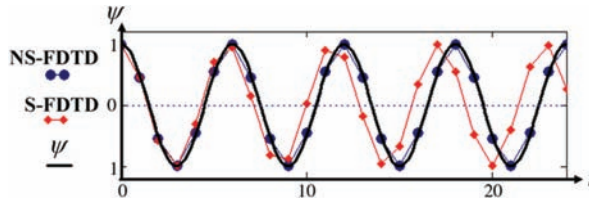


Figure 3.2 Analytic solution ψ versus numerical solutions. S-FDTD is conventional second-order FDTD [Eq. (3.9)], and NS-FDTD is the algorithm [Eq. (3.25)]; T = oscillator period = $6\Delta t$.

3.5 Analytical Solutions of the Forced Damped Harmonic Oscillator

3.5.1 Free damped oscillator

Let us now examine a more complicated system. The equation of motion for the damped harmonic oscillator is

$$(\partial_t^2 + 2\alpha\partial_t + \omega^2)\psi(t) = 0. \quad (3.28)$$

For algebraic convenience, it is conventional to insert a factor of 2 in front of α . Inserting the ansatz $\psi(t) = e^{wt}$ into Eq. (3.28) and solving for w , we find that $w = w_{\pm}$, where

$$w_{\pm} = -\alpha \pm i\sqrt{\omega^2 - \alpha^2}. \quad (3.29)$$

The condition $0 \leq \alpha \leq \omega$ yields damped oscillatory solutions. The general solution of Eq. (3.28) is thus

$$\psi(t) = a_+ e^{(i\omega' - \alpha)t} + a_- e^{(-i\omega' - \alpha)t}, \quad (3.30a)$$

or

$$\psi(t) = [a_s \sin(\omega't) + a_c \cos(\omega't)]e^{-\alpha t}, \quad (3.30b)$$

where

$$\omega'^2 = \omega^2 - \alpha^2. \quad (3.31)$$

3.5.2 Forced damped oscillator

The equation of motion for the forced damped harmonic oscillator is

$$(\partial_t^2 + 2\alpha\partial_t + \omega^2)\psi(t) = s(t), \quad (3.32)$$

where $s(t)$ is a driving force that is turned on at $t = 0$, so $s(t < 0) = 0$. At $t \leq 0$, the oscillator is at rest in its equilibrium position:

$$\psi(t) = 0 \text{ for } t \leq 0, \quad (3.33a)$$

$$\partial_t \psi(t) = 0 \text{ for } t \leq 0. \quad (3.33b)$$

Equation (3.32) can be solved analytically in terms of a Green's function G , which satisfies both

$$(\partial_t^2 + 2\alpha\partial_t + \omega^2)G(t - t') = \delta(t - t') \quad (3.34)$$

and the initial conditions of Eq. (3.33). In Appendix 3.3, it is shown that

$$G(t - t') = \Theta(t - t') e^{-\alpha(t-t')} \frac{\sin[\omega'(t - t')]}{\omega'}, \quad (3.35)$$

where Θ is the step function (see Appendix 3.4). The solution of Eq. (3.32) with the initial conditions of Eq. (3.33) is

$$\begin{aligned} \psi(t) &= \int_{-\infty}^{\infty} dt' s(t') G(t - t') \\ &= \frac{e^{-\alpha t}}{\omega'} \int_0^t dt' e^{\alpha t'} \sin[\omega'(t - t')] s(t'). \end{aligned} \quad (3.36)$$

Driving force turned on instantaneously

For example, if $s(t) = \Theta(t) e^{i\omega_0 t}$, then

$$\psi(t) = \frac{e^{i\omega_0 t}}{\omega^2 - \omega_0^2 + 2i\alpha\omega_0} + \frac{e^{-\alpha t}}{2i\omega'} \left[\frac{e^{-i\omega' t}}{\alpha + i(\omega_0 + \omega')} - \frac{e^{i\omega' t}}{\alpha + i(\omega_0 - \omega')} \right] \quad (3.37a)$$

for $t \geq 0$, and

$$\psi(t) = 0 \quad (3.37b)$$

for $t < 0$.

For later reference (in Section 4.4.3), we note that both terms in Eq. (3.37a) satisfy Eq. (3.32) for $s(t) = \Theta(t) e^{i\omega_0 t}$, but it is the $e^{-\alpha t}$ term, which vanishes for $\alpha t \gg 0$, that enforces the initial conditions of Eq. (3.33).

If $\omega_0 = \omega$, the oscillations are large and the oscillator is said to be in resonance with the driving force; if $\alpha = 0$, the amplitude of the oscillations grows to infinity.

Driving force turned on slowly

In FDTD calculations, driving forces that are suddenly turned on can give rise to large errors. Including a slow turn-on function in the source, we have $s(t) = \Theta(t) (1 - e^{-\beta t}) e^{i\omega_0 t}$, and we need to solve

$$(\partial_t^2 + 2\alpha \partial_t + \omega^2) \psi(t) = \Theta(t) (1 - e^{-\beta t}) e^{i\omega_0 t}. \quad (3.38)$$

The solution of Eq. (3.38) is

$$\psi_e = \psi_0 - \Delta\psi_e, \quad (3.39)$$

where ψ_0 is defined to be the right side of Eq. (3.37), and $\Delta\psi_e$ is the solution of

$$(\partial_t^2 + 2\alpha \partial_t + \omega^2) \Delta\psi_e(t) = \Theta(t) e^{i(\omega_0 + i\beta)t}. \quad (3.40)$$

Replacing ω_0 by $\omega_0 + i\beta$ in Eq. (3.37), we find that

$$\Delta\psi_e(t) = \frac{e^{-\beta t} e^{i\omega_0 t}}{\omega^2 - \omega_0^2 + \beta^2 + 2i(\alpha - \beta)\omega_0} + \frac{e^{-\alpha t}}{2i\omega'} \left[\frac{e^{-i\omega' t}}{\alpha - \beta + i(\omega_0 + \omega')} - \frac{e^{i\omega' t}}{\alpha - \beta + i(\omega_0 - \omega')} \right] \quad (3.41)$$

for $t \geq 0$, and $\Delta\psi_e = 0$ for $t < 0$.

3.6 Forced Damped Harmonic Oscillator: Standard Finite Difference Models

We now construct FD models of the forced damped harmonic oscillator:

$$(\partial_t^2 + 2\alpha \partial_t + \omega^2)\psi(t) = s(t). \quad (3.42)$$

We approximate the second derivative by $\partial_t^2\psi(t) \cong d_t^2\psi(t)/\Delta t^2$. There are three possible models of the first derivative: the standard forward (SF) FD approximation,

$$\partial_t\psi(t) \cong \frac{d_t^f\psi(t)}{\Delta t}, \quad (3.43)$$

where $d_t^f\psi(t) = \psi(t + \Delta t) - \psi(t)$; the standard backward (SB) FD approximation,

$$\partial_t\psi(t) \cong \frac{d_t^b\psi(t)}{\Delta t}, \quad (3.44)$$

where $d_t^b\psi(t) = \psi(t) - \psi(t - \Delta t)$; and the double-step standard central (SC) FD approximation,

$$\partial_t\psi(t) = \frac{d_t^{c,2}\psi(t)}{2\Delta t}, \quad (3.45)$$

where $d_t^{c,2}\psi(t) = \psi(t + \Delta t) - \psi(t - \Delta t)$.

Using the SF-FD approximation, the SF-FD model becomes

$$(d_t^2 + 2\alpha \Delta t d_t^f + \omega^2 \Delta t^2)\psi(t) = \Delta t^2 s(t), \quad (3.46a)$$

or

$$\psi_{\tau+1} - \frac{2 + 2\alpha \Delta t - \omega^2 \Delta t^2}{1 + 2\alpha \Delta t} \psi_{\tau} + \frac{1}{1 + 2\alpha \Delta t} \psi_{\tau-1} = \frac{1}{1 + 2\alpha \Delta t} \Delta t^2 s_{\tau}, \quad (3.46b)$$

and the SF-FDTD algorithm becomes

$$\psi_{\tau+1} = -\frac{1}{1 + 2\alpha \Delta t} \psi_{\tau-1} + \frac{2 + 2\alpha \Delta t - \omega^2 \Delta t^2}{1 + 2\alpha \Delta t} \psi_{\tau} + \frac{1}{1 + 2\alpha \Delta t} \Delta t^2 s_{\tau}. \quad (3.47)$$

Similarly, the SB-FD model is

$$\psi_{\tau+1} + (1 - 2\alpha \Delta t) \psi_{\tau-1} - (2 - 2\alpha \Delta t - \omega^2 \Delta t^2) \psi_{\tau} = \Delta t^2 s_{\tau}, \quad (3.48)$$

and the SB-FDTD algorithm is

$$\psi_{\tau+1} = -(1 - 2\alpha \Delta t) \psi_{\tau-1} + (2 - 2\alpha \Delta t - \omega^2 \Delta t^2) \psi_{\tau} + \Delta t^2 s_{\tau}. \quad (3.49)$$

Using the SC-FD approximation, the SC-FD model is

$$(d_t^2 + \omega^2 \Delta t^2 + \alpha \Delta t d_t^{c,2}) \psi(t) = \Delta t^2 s(t), \quad (3.50)$$

or

$$\psi_{\tau+1} - \frac{2 - \omega^2 \Delta t^2}{1 + \alpha \Delta t} \psi_{\tau} + \frac{1 - \alpha \Delta t}{1 + \alpha \Delta t} \psi_{\tau-1} = \frac{1}{1 + \alpha \Delta t} \Delta t^2 s_{\tau}, \quad (3.51)$$

and the SC-FDTD algorithm is

$$\psi_{\tau+1} = -\frac{1 - \alpha \Delta t}{1 + \alpha \Delta t} \psi_{\tau-1} + \frac{2 - \omega^2 \Delta t^2}{1 + \alpha \Delta t} \psi_{\tau} + \frac{1}{1 + \alpha \Delta t} \Delta t^2 s_{\tau}. \quad (3.52)$$

The initial conditions of Eq. (3.33) can be modeled by

$$\psi(-\Delta t) = \psi(0) = 0. \quad (3.53)$$

In Fig. 3.3 we compare SF-, SB-, and SC-FDTD calculations with the analytic solution of a forced damped harmonic oscillator and find that the SF-FDTD algorithm is the most accurate, while the SB-FDTD is the least accurate. The larger the value of α the more accurate the SF-FDTD is relative to the SC-FDTD.

Following the methods of Appendix 3.1, the stability conditions of these algorithms can be determined. Since the derivation is quite tedious, we omit it.

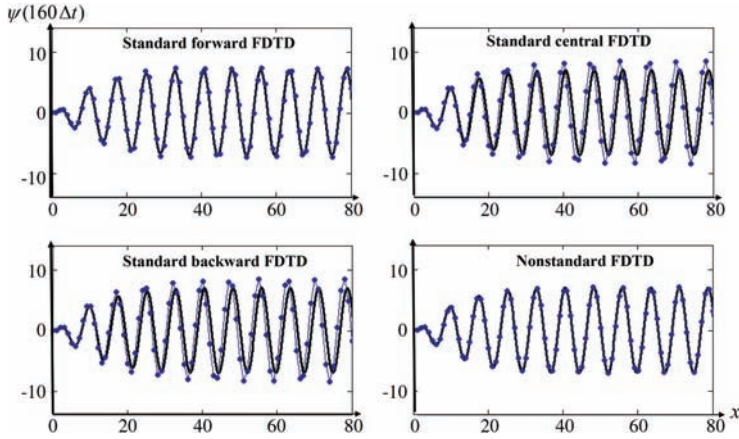


Figure 3.3 Forced damped harmonic oscillator calculations showing the analytic solution (solid line) versus numerical solutions computed using standard forward, standard backward, standard central, and nonstandard FDTD after 160 time steps; $T/\Delta t = 8$, $\omega = 1.05\omega_0$, and $\alpha = \omega = 0.1\omega_0$.

3.7 Forced Damped Harmonic Oscillator: Nonstandard Finite Difference Models

3.7.1 No driving force

Replacing $\omega\Delta t$ with $\tilde{\omega}_f$ and $\alpha\Delta t$ with $\tilde{\alpha}_f$ in the SF-FD model, Eq. (3.46a) gives the nonstandard (NS) F-FD model,

$$(d_t^2 + 2\tilde{\alpha}_f d_t^f + \tilde{\omega}_f^2)\psi(t) = 0, \quad (3.54a)$$

or

$$\psi_{\tau+1} - \left(\frac{2 + 2\tilde{\alpha}_f - \tilde{\omega}_f^2}{1 + 2\tilde{\alpha}_f} \right) \psi_\tau + \left(\frac{1}{1 + 2\tilde{\alpha}_f} \right) \psi_{\tau-1} = 0. \quad (3.54b)$$

Similarly, $\omega\Delta t \rightarrow \tilde{\omega}_f$ and $\alpha\Delta t \rightarrow \tilde{\alpha}_f$ in the SB-FD model yields the NSB-FD model,

$$(d_t^2 + \tilde{\omega}_c^2 + \tilde{\alpha}_c d_t^f)\psi(t) = 0, \quad (3.55a)$$

or

$$\psi_{\tau+1} + (1 - 2\alpha\Delta t)\psi_{\tau-1} - (2 - 2\alpha\Delta t - \omega^2\Delta t^2)\psi_\tau = 0. \quad (3.55b)$$

The NSC-FD model, obtained by putting $\omega\Delta t \rightarrow \tilde{\omega}_c$ and $\alpha\Delta t \rightarrow \tilde{\alpha}_c$ in the SC-FD model, is

$$(d_t^2 + \tilde{\omega}_c^2 + \tilde{\alpha}_c d_t^{c,2})\psi(t) = 0, \quad (3.56a)$$

or

$$\psi_{\tau+1} - \left(\frac{2 - \tilde{\omega}_c^2}{1 + \tilde{\alpha}_c}\right)\psi_\tau + \left(\frac{1 - \tilde{\alpha}_c}{1 + \tilde{\alpha}_c}\right)\psi_{\tau-1} = 0. \quad (3.56b)$$

The NSF-FD, NSB-FD, and NSC-FD models all have the same form:

$$\psi_{\tau+1} - B \psi_\tau + C \psi_{\tau-1} = 0. \quad (3.57)$$

Substituting the solution of the damped SHO, $\psi_\pm(t) = e^{(\pm i\omega' - \alpha)t}$, into Eq. (3.57), and requiring that the left side vanish for both ψ_+ and ψ_- , we find that

$$B = 2e^{-\alpha\Delta t} \cos(\omega'\Delta t), \quad (3.58a)$$

$$C = e^{-2\alpha\Delta t}. \quad (3.58b)$$

Thus, an exact NS-FD model of the damped SHO is

$$\psi_{\tau+1} - 2\cos(\omega'\Delta t) e^{-\alpha\Delta t} \psi_\tau + e^{-2\alpha\Delta t} \psi_{\tau-1} = 0. \quad (3.59)$$

While the S-FD models differ according to how $\partial_t\psi$ is modeled, the NS-FD models are all the same, regardless of which FD approximation is used to model $\partial_t\psi$. The NS-FDTD algorithm

$$\psi_{\tau+1} = -e^{-2\alpha\Delta t} \psi_{\tau-1} + 2\cos(\omega'\Delta t) e^{-\alpha\Delta t} \psi_\tau \quad (3.60)$$

is thus exact.

From Eq. (3.58), we find that

$$\tilde{\alpha}_f = \frac{e^{2\alpha\Delta t} - 1}{2} \quad (3.61a)$$

$$= e^{\alpha\Delta t} \sinh(\alpha\Delta t),$$

$$\tilde{\alpha}_c = \tanh(\alpha\Delta t), \quad (3.61b)$$

$$\tilde{\omega}_f^2 = 1 + 4e^{\alpha\Delta t} \sin^2(\omega'\Delta t/2), \quad (3.62a)$$

$$\tilde{\omega}_c^2 = \frac{4 \left[\sin^2(\omega'\Delta t/2) + \sinh^2(\alpha\Delta t/2) \right]}{\cosh(\alpha\Delta t)}. \quad (3.62b)$$

Noting that for small $\alpha\Delta t$, $e^{-2\alpha\Delta t} = e^{-\alpha\Delta t}/e^{\alpha\Delta t} \cong (1 - \alpha\Delta t)/(1 + \alpha\Delta t)$, it is easy to confirm that the NS-FD model reduces to the S-FFD and S-CFD models for $\alpha\Delta t$ and $\omega'\Delta t$.

3.7.2 NS-FD model for the forced damped harmonic oscillator

We are now ready to derive an exact NS-FD model of the forced damped harmonic oscillator. We postulate a model of the form

$$\psi_{\tau+1} - B\psi_{\tau} + C\psi_{\tau-1} = A\Delta t^2 s_{\tau}, \quad (3.63)$$

where A is a constant to be determined, with B and C given by Eq. (3.58).

The difference equation [Eq. (3.63)] can be solved in terms of a discrete Green's function (DGF) $g_{\tau-\tau'}$ (see Appendix 3.5), which satisfies

$$g_{\tau+1-\tau'} - Bg_{\tau-\tau'} + Cg_{\tau-1-\tau'} = \delta_{\tau-\tau',0}, \quad (3.64)$$

and

$$g_{\tau-\tau'} = 0 \text{ for } \tau - \tau' \leq 0. \quad (3.65)$$

In terms of the DGF, its solution is

$$\varphi_{\tau} = A\Delta t^2 \sum_{\tau'=0}^{\infty} s_{\tau'} g_{\tau-\tau'}. \quad (3.66)$$

Here we write ψ to denote the solution of the forced damped harmonic oscillator (differential equation) and φ to denote the solution of its FD model, (difference equation) Eq. (3.63).

As shown in Appendix (3.5),

$$g_{\tau-\tau'} = \Theta(\tau - \tau') \frac{r_+^{\tau-\tau'} - r_-^{\tau-\tau'}}{r_+ - r_-}, \quad (3.67)$$

where $r_{\pm}$ are the roots of $z^2 - Bz + C = 0$, and

$$r_{\pm} = \frac{1}{2}(B \pm \sqrt{B^2 - 4C}) = e^{-\alpha\Delta t} e^{\pm i\omega'\Delta t}. \quad (3.68)$$

Since $|r_{\pm}| \leq 1$, the NS-FDTD algorithm for the damped harmonic oscillator is numerically stable. For $|r_{\pm}| < 1$, the algorithm is oscillatory with a constant amplitude.

Next, using Eq. (3.68) in Eq. (3.67), the DGF becomes

$$g_{\tau-\tau'} = \Theta(\tau - \tau') \frac{e^{\alpha\Delta t}}{\sin(\omega'\Delta t)} \frac{\sin[\omega'(\tau - \tau')\Delta t]}{e^{\alpha(\tau-\tau')\Delta t}}, \quad (3.69)$$

and the solution of the forced damped harmonic oscillator FD model [Eq. (3.63)] is thus

$$\varphi_\tau = A \Delta t^2 \frac{e^{\alpha \Delta t}}{\sin(\omega' \Delta t)} \left\{ \sum_{\tau'=0}^{\tau-1} s_{\tau'} \frac{\sin[\omega'(\tau - \tau') \Delta t]}{e^{\alpha[\tau - \tau'] \Delta t}} \right\} \quad (3.70a)$$

$$= A \frac{\Delta t e^{\alpha \Delta t}}{\sin(\omega' \Delta t)} e^{-\alpha \tau \Delta t} \sum_{\tau'=0}^{\tau-1} \Delta t s(\tau' \Delta t) e^{\alpha \Delta t \tau'} \sin[\omega'(\tau - \tau') \Delta t]. \quad (3.70b)$$

We now seek A such that φ , the solution of the difference equation [Eq. (3.63)], is identical to ψ , the solution of the differential equation [Eq. (3.42)]. In the limit $\Delta t \rightarrow 0$, the summation in Eq. (3.70b) becomes an integral; hence,

$$\varphi(t) = A \frac{e^{\alpha \Delta t}}{\Delta t \sin(\omega' \Delta t)} e^{-\alpha t} \int_0^t dt' s(t') e^{\alpha t'} \sin[\omega'(t - t')]. \quad (3.71)$$

Comparing φ with ψ , given by

$$\psi(t) = \frac{e^{-\alpha t}}{\omega'} \int_0^t dt' s(t') e^{\alpha t'} \sin[\omega'(t - t')], \quad (3.72)$$

we see that the choice

$$A = \frac{\sin(\omega' \Delta t)}{\Delta t \omega' e^{\alpha \Delta t}} \quad (3.73)$$

in Eq. (3.71) gives $\varphi(t) = \psi(t)$. For example, if $T = 8\Delta t$ (implying that $\omega\Delta t = \pi/4$) and $\alpha = 0$ (implying that $\omega' = \omega$), we find that $A = 2\sqrt{2}/\pi \cong 0.90$.

Thus, an exact NS-FD model of the forced damped harmonic oscillator is

$$\psi_{\tau+1} - 2 \frac{\cos(\omega' \Delta t)}{e^{\alpha \Delta t}} \psi_\tau + \frac{1}{e^{2\alpha \Delta t}} \psi_{\tau-1} = \frac{\Delta t \sin(\omega' \Delta t)}{\omega' e^{\alpha \Delta t}} s_\tau. \quad (3.74)$$

In Fig. 3.3 we compared NS- and S-FDTD calculations with the analytic solution of

$$(\partial_t^2 + 2\alpha \partial_t + \omega^2)\psi(t) = \Theta(t) \cos(\omega t). \quad (3.75)$$

In the undamped case ($\alpha = 0$), $\omega' = \omega$, $C = 1$, $B = 2\cos(\omega\Delta t)$, and the NS-FD model of the forced harmonic oscillator is

$$\psi_{\tau+1} - 2 \cos(\omega\Delta t) \psi_\tau + \psi_{\tau-1} = \frac{\Delta t \sin(\omega\Delta t)}{\omega} s_\tau, \quad (3.76a)$$

or, equivalently,

$$[d_t^2 + 4 \sin^2(\omega \Delta t/2)]\psi(t) = \frac{\sin(\omega \Delta t)}{\omega} \Delta t s(t). \quad (3.76b)$$

In the limit $\Delta t \rightarrow 0$, the NS-FD model converges to the S-FD model, but when Δt is not infinitesimal, the NS-FD model is much more accurate than the S-FD model.

Important Points of Chapter 3

- We introduce the standard (S) and nonstandard (NS) FDTD methodology for the harmonic oscillator and its variants.
- Fourth-order FDTD used to solve a second-order differential equation is numerically unstable.
- If the number of initial conditions needed to iterate an FDTD algorithm is greater than the number of initial conditions needed to specify a solution of the differential equation (that it is supposed to solve), the FDTD algorithm may be numerically unstable and yield spurious solutions.
- There exist exact nonstandard (NS) FDTD algorithms to solve the harmonic oscillator.
- We derive Green's functions for the SHO differential equation and for its corresponding difference equation.

Appendix 3.1 Stability Analysis of the Second-Order Finite Difference Model

Analysis 1

The (equivalent) difference equations [Eqs. (3.5) and (3.8)], repeated below,

$$(d_t^2 + \omega^2 \Delta t^2)\psi(t) = 0, \quad (A3.1.1)$$

$$\psi_{\tau+1} + \psi_{\tau-1} - (2 - \omega^2 \Delta t^2)\psi_\tau = 0, \quad (A3.1.2)$$

can be solved analytically.

To solve Eq. (A3.1.1), we postulate a solution of the form $\psi(t) = e^{i\omega' t}$. Using the fact that

$$\frac{d_t^2 e^{i\omega' t}}{e^{i\omega' t}} = -4 \sin^2(\omega \Delta t/2), \quad (A3.1.3)$$

we find that

$$4 \sin^2(\omega' \Delta t/2) = \omega^2 \Delta t^2, \quad (A3.1.4)$$

and hence,

$$\omega' \Delta t = 2 \arcsin(\omega \Delta t/2). \quad (A3.1.5)$$

The argument of $\arcsin x$ is constrained by $-1 \leq x \leq 1$, which implies the constraint

$$-2 \leq \omega \Delta t \leq 2, \quad (\text{A3.1.6a})$$

or

$$\frac{T}{\Delta t} \geq \pi, \quad (\text{A3.1.6b})$$

where $T = 2\pi/|\omega|$ is the oscillation period. If Eq. (A3.1.6) is violated, ω' is complex, there is an exponentially growing solution, and the algorithm becomes numerically unstable.

An exponentially rising solution does not *per se* imply instability, but here it does because the physical solution we seek consists of oscillations of constant amplitude. For example, if $T/\Delta t = \pi/2$ (implying that $\omega\Delta t = 4$), then [using Eq. (A3.2.17) in Note A3.2.1 below], we find that

$$\omega'\Delta t = \pi + i 2 \ln(1 + \sqrt{5}). \quad (\text{A3.1.7})$$

Expanding Eq. (A3.1.5) in a Taylor series, we find that the angular frequency ω' of the S-FD solution deviates from the angular frequency ω of the simple harmonic oscillator by

$$\begin{aligned} \frac{\omega' - \omega}{\omega} &= \frac{2 \arcsin(\omega\Delta t/2)}{\omega\Delta t} - 1 \\ &= \frac{1}{24} \omega^2 \Delta t^2 + \frac{3}{640} \omega^4 \Delta t^4 + \dots \end{aligned} \quad (\text{A3.1.8})$$

The general solution of Eq. (A3.1.1) can be cast into the form

$$\psi(t) = a \cos(\omega' t) + b \sin(\omega' t), \quad (\text{A3.1.9})$$

where a and b are constants determined by the initial conditions. Imposing the initial conditions

$$\psi_0 = \psi(0), \quad (\text{A3.1.10a})$$

$$\psi_1 = \psi_0 \cos(\omega\Delta t), \quad (\text{A3.1.10b})$$

we find that

$$a = \psi_0, \quad (\text{A3.1.11a})$$

$$b = \psi_0 \frac{\cos(\omega\Delta t) - \cos(\omega'\Delta t)}{\sin(\omega'\Delta t)}. \quad (\text{A3.1.11b})$$

Obviously, as $\omega\Delta t \rightarrow 0$, the solution of this FD model converges to the analytic solution of the harmonic oscillator.

Analysis 2

An alternative approach is to substitute a solution of the form $\psi_\tau = \lambda^\tau$ into Eq. (A3.1.2) to obtain

$$\lambda^2 - (2 - \omega^2 \Delta t^2) \lambda + 1 = 0, \quad (\text{A3.1.12})$$

which has the solutions $\lambda = \lambda_\pm$, where

$$\lambda_\pm = b \pm \sqrt{b^2 - 1}, \quad (\text{A3.1.13})$$

where

$$b = 1 - \omega^2 \Delta t^2 / 2. \quad (\text{A3.1.14})$$

The general solution is

$$\psi_\tau = a_+ \lambda_+^\tau + a_- \lambda_-^\tau, \quad (\text{A3.1.15})$$

where the $a_\pm$ values are determined by the initial conditions.

Since solutions of the harmonic oscillator are constant amplitude harmonic oscillations, we require the $\lambda_\pm$ values to be complex and of unit magnitude. Complex $\lambda_\pm$ implies the condition

$$b^2 < 1, \quad (\text{A3.1.16})$$

which gives

$$\lambda_\pm = b \pm i\sqrt{1 - b^2}, \quad (\text{A3.1.17})$$

and

$$|\lambda_\pm| = 1; \quad (\text{A3.1.18})$$

hence, $\lambda_\pm = e^{\pm i \omega'}$, where $\sin(\omega') = \sqrt{1 - b^2}$. The condition given by Eq. (A3.1.16) is equivalent to the constraint given by Eq. (A3.1.6).

Appendix 3.2 Stability Analysis of the Fourth-Order Finite Difference Model

Analysis 1

The fourth-order FD model of the SHO is

$$\left[d_t^2 - \frac{1}{12} d_t^4 + \omega^2 \Delta t^2 \right] \psi_\tau = 0, \quad (\text{A3.2.1})$$

or

$$-(\psi_{\tau+2} + \psi_{\tau-2}) + 16(\psi_{\tau+1} + \psi_{\tau-1}) - (30 - 12\omega^2 \Delta t^2) \psi_\tau = 0. \quad (\text{A3.2.2})$$

Following Analysis 1 in Appendix 3.1, postulating a solution of the form $\psi(t) = e^{i\omega' t}$, and using Eq. (A3.1.3), we obtain

$$4 \sin^4(\omega' \Delta t / 2) + 12 \sin^2(\omega' \Delta t / 2) - 3\omega^2 \Delta t^2 = 0. \quad (\text{A3.2.3})$$

Solving for $\sin^2(\omega' \Delta t / 2)$, we find two solutions, ω'_1 and ω'_2 , where

$$\sin^2(\omega'_1 \Delta t / 2) = \frac{3}{2} \left(\sqrt{1 + \omega^2 \Delta t^2 / 3} - 1 \right), \quad (\text{A3.2.4a})$$

and

$$\sin^2(\omega'_2 \Delta t / 2) = i \sin^2(\omega'_1 \Delta t / 2). \quad (\text{A3.2.4b})$$

Assuming ω'_1 to be real in Eq. (A3.2.4a), we obtain

$$\omega'_1 \Delta t = \pm 2 \arcsin \left[\sqrt{\frac{3}{2}} \left(\sqrt{1 + \omega^2 \Delta t^2 / 3} - 1 \right)^{1/2} \right]. \quad (\text{A3.2.5})$$

This implies the numerical stability constraint,

$$\sqrt{2} \leq \omega \Delta t \leq \sqrt{22/3}, \quad (\text{A3.2.6a})$$

$$2.320 \cong \frac{2\pi}{\sqrt{22/3}} \leq \frac{T}{\Delta t} \leq \frac{2\pi}{\sqrt{2}} \cong 4.443. \quad (\text{A3.2.6b})$$

Expanding Eq. (A3.2.5) in a Taylor series, we find that the angular frequency ω'_1 , given by the solution equation [Eq. (A3.2.4a)], deviates from the true angular frequency ω of the SHO by

$$\begin{aligned} \frac{\omega'_1 - \omega}{\omega} &= \frac{2}{\omega \Delta t} \arcsin \left[\sqrt{\frac{3}{2}} \left(\sqrt{1 + \omega^2 \Delta t^2 / 3} - 1 \right)^{1/2} \right] - 1 \\ &= \frac{1}{180} \omega^4 \Delta t^4 + \frac{1}{2016} \omega^6 \Delta t^6 + \dots \end{aligned} \quad (\text{A3.2.7})$$

The deviation of ω'_1 from ω is proportional to $(\omega \Delta t)^4$ in Eq. (A3.2.7) for the fourth-order FD model. On the other hand, the deviation of ω' from ω in Eq. (3.1.8) is proportional to $(\omega \Delta t)^2$. We might therefore suppose that the fourth-order FD model given by Eq. (A3.2.1) is better than the second-order FD model given by Eq. (A3.1.1). Although the solution of the fourth-order model apparently converges to the analytic solution of the harmonic oscillator, we cannot actually let $\omega \Delta t \rightarrow 0$ because there is a minimum stable value for $\omega \Delta t$. In addition, we have the solution given by Eq. (A3.2.4b), which is a source of trouble.

Solution (A3.2.4b) gives

$$\sin(\omega'_2 \Delta t/2) = \pm e^{i\pi/4} \sin(\omega'_1 \Delta t/2), \quad (\text{A3.2.8})$$

and hence (see Note A3.2.1), ω'_2 is complex.

Setting $a^2 = 2 \sin^2(\omega'_1 \Delta t/2)$, Eq. (A3.2.4a) gives $0 \leq a \leq \sqrt{2}/2$. Since $\text{Re}(\omega'_2 \Delta t)$ is real, we choose the “−” sign in Eq. (A3.2.13a) to obtain

$$\sin^2[\text{Re}(\omega'_2 \Delta t/2)] = a^2 - \frac{1}{2} \left(\sqrt{1 + 4a^4} - 1 \right), \quad (\text{A3.2.9a})$$

$$\sinh^2[\text{Im}(\omega'_2 \Delta t/2)] = a^2 + \frac{1}{2} \left(\sqrt{1 + 4a^4} - 1 \right). \quad (\text{A3.2.9b})$$

Because $\text{Im}(\omega'_2 \Delta t/2) \neq 0$, Eq. (A3.2.8) implies an exponentially rising solution to Eq. (A3.2.1), which gives rise to numerical instability for all values of $\omega \Delta t$.

Analysis 2

Following Analysis 2 for the second-order case, we postulate the solution of Eq. (A3.2.2) to be $\psi_\tau = \lambda^\tau$ and obtain

$$\lambda^4 - 16\lambda^3 + (30 - 12\omega^2 \Delta t^2)\lambda^2 - 16\lambda + 1 = 0, \quad (\text{A3.2.10})$$

which has the solutions

$$\lambda_{1\pm} = 4 - \sqrt{3\omega^2 \Delta t^2 + 9} \pm i\sqrt{8\sqrt{3\omega^2 \Delta t^2 + 9} - (3\omega^2 \Delta t^2 + 24)}, \quad (\text{A3.2.11a})$$

$$\lambda_{2\pm} = 4 + \sqrt{3\omega^2 \Delta t^2 + 9} \pm \sqrt{8\sqrt{3\omega^2 \Delta t^2 + 9} + (3\omega^2 \Delta t^2 + 24)}. \quad (\text{A3.2.11b})$$

The general solution of Eq. (A3.2.2) is

$$\psi_\tau = a_{1+}\lambda_{1+}^\tau + a_{1-}\lambda_{1-}^\tau + a_{2+}\lambda_{2+}^\tau + a_{2-}\lambda_{2-}^\tau, \quad (\text{A3.2.12})$$

where the $a_{1,2\pm}$ values are determined by the initial conditions.

Because $|\lambda_{1\pm}| = 1$, $\lambda_{1\pm}^\tau$ does not diverge, but $\lambda_{2+} > 1$ for all values of $\omega \Delta t$. Thus, a fourth-order FDTD algorithm derived from the FD model [Eq. (A3.3.2)] is unconditionally unstable.

One might suppose that if the initial conditions were such that $a_{2+} = 0$, the algorithm would be stable, but this is not the case because small round-off and truncation errors in the computation will give produce intermediate solutions for which $a_{2+} \neq 0$ (see Section 2.4.4).

Note A3.2.1

With some rather tedious algebra, it can be shown that if

$$\sin(x + iy) = a + ib, \quad (\text{A3.2.13})$$

then

$$2 \sin^2 x = 1 + a^2 + b^2 \pm \sqrt{(1 + a^2 + b^2)^2 - 4a^2}, \quad (\text{A3.2.14a})$$

and

$$\sinh^2 y = a^2 + b^2 - \sin^2 x, \quad (\text{A3.2.14b})$$

where x , y , a , and b are taken to be real.

For the case where $a > 1$ and $b = 0$, we find that

$$\sin^2 x = 1, \quad (\text{A3.2.15})$$

[the “+” sign must be taken in Eq. (A3.2.13a) because the “−” sign would give $\sin^2 x = a^2 > 1$], and

$$\sinh^2 y = a^2 - 1. \quad (\text{A3.2.16})$$

If $\sinh \alpha = \beta$ for real α and β , then the inverse of $\sinh$ is given by

$$\sinh^{-1} \beta = \ln \left(\beta + \sqrt{1 + \beta^2} \right). \quad (\text{A3.2.17})$$

Thus,

$$\arcsin(a) = \frac{\pi}{2} + i \ln \left(a + \sqrt{1 + a^2} \right) \quad (\text{A3.2.18})$$

for $a > 1$.

For the case where $a = b$,

$$\sin^2 x = a^2 + \frac{1}{2} \left(1 \pm \sqrt{1 + 4a^4} \right), \quad (\text{A3.2.19a})$$

$$\sinh^2 y = a^2 + \frac{1}{2} \left(-1 \mp \sqrt{1 + 4a^4} \right). \quad (\text{A3.2.19b})$$

Appendix 3.3 Green's Function for the Damped Harmonic Oscillator

A3.3.1 Simple harmonic oscillator without damping

A SHO driven by an external force $s(t)$ obeys the equation

$$(\partial_t^2 + \omega^2)\psi(t) = s(t). \quad (\text{A3.3.1})$$

Its solution can be expressed in terms of what is called a Green's function, which satisfies

$$(\partial_t^2 + \omega^2)G(t, t') = \delta(t - t') \quad (\text{A3.3.2})$$

and the initial conditions of the problem we wish to solve. The Green's function gives the response at time t to a δ function impulse (see Appendix 3.4) force applied at time t' . It must satisfy not only Eq. (A3.3.2), but also the initial conditions.

Using the properties of the δ function, it can be shown that

$$\psi(t) = \int_{-\infty}^{\infty} dt' s(t') G(t - t'). \quad (\text{A3.3.3})$$

Before the driving force is turned on at $t = 0$, let the oscillator be at rest in its equilibrium position so that

$$\psi(t) = 0 \quad \text{for } t \leq 0, \quad (\text{A3.3.4a})$$

$$\partial_t \psi(t) = 0 \quad \text{for } t \leq 0. \quad (\text{A3.3.4b})$$

It is reasonable to suppose that G is a function only of the difference $\tau = t - t'$ so that $G(t, t') = G(t - t')$ and Eq. (A3.3.2) becomes

$$(\partial_\tau^2 + \omega^2)G(\tau) = \delta(\tau). \quad (\text{A3.3.5})$$

For $\tau = t - t' < 0$, the conditions of Eq. (A3.3.4) become

$$G(\tau) = 0 \quad \text{for } \tau \leq 0, \quad (\text{A3.3.6a})$$

$$\partial_\tau G(0) = 0 \quad \text{for } \tau < 0. \quad (\text{A3.3.6b})$$

While $G(\tau)$ must be continuous at $\tau = 0$ so that $\partial_\tau G(0)$ exists (is finite), $\partial_\tau G(\tau)$ is not continuous at $\tau = 0$ because $\partial_\tau^2 G(0)$ is infinite due to the δ function in Eq. (A3.3.5). For this reason, we take $\tau < 0$ in Eq. (A3.3.6b) and $\tau \leq 0$ in Eq. (A3.3.6a).

Since for $\tau > 0$, G satisfies the free harmonic oscillator equation

$$\left(\frac{d^2}{d\tau^2} + \omega^2 \right) G(\tau) = 0 \quad (\text{A3.3.7})$$

and the initial conditions of Eq. (A3.3.6), we postulate a solution of the form

$$G(\tau) = A \Theta(\tau) \sin(\omega\tau), \quad (\text{A3.3.8})$$

where A is a constant to be determined. Integrating both sides of Eq. (A3.3.5) gives

$$\int_{-\eta}^{+\eta} d\tau \left(\partial_{\tau}^2 + \omega^2 \right) G(\tau) = 1. \quad (\text{A3.3.9})$$

Evaluating the integral in the limit $0 < \eta \rightarrow 0$, the continuity of $G(\tau)$ and the discontinuity of $\partial_{\tau}G(\tau)$ at $\tau = 0$ give

$$\lim_{\eta \rightarrow 0} [G(\eta) - G(-\eta)] = 0, \quad (\text{A3.3.10})$$

$$\lim_{\eta \rightarrow 0} [\partial_{\tau}G(+\eta) - \partial_{\tau}G(-\eta)] = 1. \quad (\text{A3.3.11})$$

Applying the initial conditions [Eqs. (A3.3.6b) to (A3.3.11)], we find that $A\omega = 1$, and

$$A = 1/\omega. \quad (\text{A3.3.12})$$

Thus, the Green's function for a forced SHO initially at rest in equilibrium is

$$G(t - t') = \Theta(t - t') \frac{1}{\omega} \sin[\omega(t - t')]. \quad (\text{A3.3.13})$$

Using Eq. (A3.4.28) (in Appendix 3.4), it can be verified that Eq. (A3.3.13) is the solution of Eq. (A3.3.5).

A3.3.2 Simple harmonic oscillator with damping

Again assuming that $G(t, t') = G(t - t')$, the Green's function for the damped harmonic oscillator satisfies

$$(\partial_t^2 + 2\alpha \partial_t + \omega^2) G(t - t') = \delta(t - t'), \quad (\text{A3.3.14})$$

where $0 \leq \alpha < \omega$, and G satisfies the initial conditions of the problem we wish to solve. For the initial conditions given in Eq. (A3.3.4), the initial conditions for this Green's function are the same as Eq. (A3.3.6) for the undamped case. Following the development for the free damped harmonic oscillator, we postulate a solution of the form

$$G(\tau) = A \Theta(\tau) e^{-\alpha \tau} \sin(\omega' \tau), \quad (\text{A3.3.15})$$

where $\omega'^2 = \omega^2 - \alpha^2$, and A is to be determined.

Integrating Eq. (A3.3.14) on the range $-\eta \leq \tau \leq \eta$, where $\eta > 0$, we obtain

$$\partial_{\tau}G(\tau)|_{\tau=-\eta}^{+\eta} + 2\alpha G(\tau)|_{\tau=-\eta}^{+\eta} + 2\eta\omega^2 G(0) = 1. \quad (\text{A3.3.16})$$

Again applying the boundary conditions of Eq. (A3.3.6), using continuity of $G(\tau)$ and the discontinuity of $\partial_{\tau}G(\tau)$ at $\tau = 0$, and taking the limit $\eta \rightarrow 0$ gives

$$\lim_{\tau \rightarrow 0^+} \partial_\tau G(\tau) = 1, \quad (\text{A3.3.17})$$

and

$$A = \frac{1}{\omega'}. \quad (\text{A3.3.18})$$

Thus,

$$G(\tau) = \Theta(\tau) e^{-\alpha\tau} \frac{\sin(\omega'\tau)}{\omega'}, \quad (\text{A3.3.19a})$$

or

$$G(t - t') = \Theta(t - t') e^{-\alpha(t-t')} \frac{\sin[\omega'(t - t')]}{\omega'}. \quad (\text{A3.3.19b})$$

Appendix 3.4 Properties of the δ Function and the Step Function

A3.4.1 δ function definition and elementary properties

The δ function is not a true function, but is what is called a distribution.² It has the following properties:

$$\delta(x) = 0 \quad \text{for } x \neq 0, \quad (\text{A3.4.1})$$

$$\int_{-\infty}^{\infty} dx \delta(x) = 1. \quad (\text{A3.4.2})$$

From Eqs. (A3.4.1) and (A3.4.2), we find that for any function f that satisfies $\lim_{x \rightarrow \pm\infty} f(x) = 0$,

$$\int_{-\infty}^{\infty} dx \delta(x) f(x) = f(0), \quad (\text{A3.4.3a})$$

or

$$\int_{-\infty}^{\infty} dx \delta(x - a) f(x) = f(a). \quad (\text{A3.4.3b})$$

Let us now evaluate $\delta(ax)$, where $a > 0$. Obviously, $\delta(ax)$ satisfies Eq. (A3.4.1). Integrating with a test function f , we find that

$$\int_{-\infty}^{\infty} dx \delta(ax) f(x) = \frac{1}{a} f(0); \quad (\text{A3.4.4})$$

thus, $\delta(ax) = \delta(x)/a$ for $a > 0$. Replacing a with $-a$ in the above integration, we find that $\delta(-ax) = \delta(x)/a$. Generalizing to $a \neq 0$,

$$\delta(ax) = \frac{1}{|a|} \delta(x). \quad (\text{A3.4.5})$$

A3.4.2 Derivative of the δ function

The derivative of the δ function can be defined by integrating it with f as

$$\int_{-\infty}^{\infty} dx \delta'(x) f(x) = \left[\delta'(x) f(x) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx \delta(x) f'(x) = -f'(0); \quad (\text{A3.4.6})$$

because $\delta(x) = 0$ for $x \neq 0$,

$$\delta'(x) = 0 \text{ for } x \neq 0. \quad (\text{A3.4.7})$$

Comparing integrands in Eq. (A3.4.6), we conclude that

$$f(x) \frac{\partial}{\partial x} \delta(x - x') = -\delta(x - x') \frac{d}{dx} f(x). \quad (\text{A3.4.8})$$

A3.4.3 Representations of the δ function

For analytic purposes, it is convenient to represent the δ function in terms of true functions. Below we give several representations that will be useful later.

Basis function expansion

A set of functions, φ_n ($n = 1, 2, \dots$), on the interval $0 \leq x \leq a$ is said to be orthonormal if

$$\langle \varphi_n | \varphi_m \rangle = \delta_{n,m}. \quad (\text{A3.4.9})$$

$\langle f | g \rangle$ denotes the inner product of functions f and g , and the Kronecker δ , $\delta_{n,m}$, is defined by $\delta_{n,m} = 1$ if $n = m$ and $\delta_{n,m} = 0$ if $n \neq m$. In general, the inner product associates two functions with a complex number. Many definitions are possible, but a commonly used definition that is useful for many purposes—including ours—is

$$\langle f | g \rangle = \int_0^a dx f^*(x) g(x), \quad (\text{A3.4.10})$$

where f^* denotes the complex conjugate of f . When $f = g$, we write $\langle f | g \rangle = \|f\|^2$, where $\|f\|$ is called the norm.

If an arbitrary function f on the interval $0 \leq x \leq a$ can be expanded in the form

$$f(x) = \sum_{n=1}^{\infty} c_n \varphi_n(x), \quad (\text{A3.4.11})$$

where

$$c_n = \langle \varphi_n | f \rangle, \quad (\text{A3.4.12})$$

and Eq. (A3.4.9) holds, then the φ_n are said to constitute a complete orthonormal set of basis functions.

Inserting Eq. (A3.4.12) into Eq. (A3.4.11), we find that

$$\begin{aligned} f(x) &= \sum_{n=1}^{\infty} \langle \varphi_n | f \rangle \varphi_n(x) \\ &= \sum_{n=1}^{\infty} \varphi_n(x) \int_0^a dx' \varphi_n^*(x') f(x') \\ &= \int_0^a dx' \left[\sum_{n=1}^{\infty} \varphi_n^*(x') \varphi_n(x) \right] f(x'). \end{aligned} \quad (\text{A3.4.13})$$

Defining both f and φ_n to vanish for x outside of $0 \leq x \leq a$, the summation $\sum_{n=1}^{\infty} \varphi_n^*(x') \varphi_n(x)$ has the same properties as the δ function with respect to integration; thus,

$$\delta(x - x') = \sum_{n=1}^{\infty} \varphi_n^*(x) \varphi_n(x'). \quad (\text{A3.4.14})$$

The 1D Helmholtz equation,

$$\left(\frac{d^2}{dx^2} + k^2 \right) \varphi(x) = 0, \quad (\text{A3.4.15})$$

has the same form as the SHO equation, but its boundary conditions are different. On the interval $0 \leq x \leq a$ with the boundary conditions

$$\varphi(0) = 0, \quad (\text{A3.4.16a})$$

$$\varphi(a) = 0, \quad (\text{A3.4.16b})$$

solutions of Eq. (A3.4.15) are

$$\varphi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x), \quad (\text{A3.4.17})$$

where

$$k_n = n \frac{\pi}{a}. \quad (\text{A3.4.18})$$

Using the definition of the inner product given by Eq. (A3.4.10), it is straightforward to demonstrate that the φ_n form an orthonormal set. The quantity $c_n = \langle \varphi_n | f \rangle$ is the Fourier sine transform of f , and the functions φ_n form a complete orthonormal set of basis functions on $0 \leq x \leq a$ with respect to the solutions of Eq. (A3.4.15) together with boundary conditions given by Eq. (A3.4.16). The δ function is thus represented by

$$\delta(x - x') = \frac{2}{a} \sum_{n=1}^{\infty} \sin(k_n x) \sin(k_n x'). \quad (\text{A3.4.19})$$

Solutions of Eq. (A3.4.15) that have the periodic boundary conditions

$$\varphi(x + a) = \varphi(x) \quad (\text{A3.4.20})$$

for $0 \leq x \leq a$ and

$$\varphi_n(x) = \frac{1}{\sqrt{a}} e^{i k_n x} \quad (\text{A3.4.21})$$

also form a complete orthonormal set of basis functions on $0 \leq x \leq a$. Thus,

$$\delta(x - x') = \frac{1}{a} \sum_{n=1}^{\infty} e^{-i k_n x} e^{-i k_n x'}. \quad (\text{A3.4.22})$$

Infinitely narrow pulse

An infinitely narrow pulse is defined by

$$\begin{aligned} d(x) &= \frac{1}{\Delta x} \quad \text{for} \quad |x| < \frac{\Delta x}{2}, \\ d(x) &= 0 \quad \text{for} \quad |x| \geq \frac{\Delta x}{2}, \end{aligned} \quad (\text{A3.4.23})$$

where $\Delta x > 0$. A representation of the δ function is

$$\delta(x) = \lim_{\Delta x \rightarrow 0} d(x). \quad (\text{A3.4.24})$$

A3.4.4 The step function

The step function is defined by

$$\begin{aligned} \Theta(x) &= 1 \quad \text{for} \quad x \geq 0, \\ \Theta(x) &= 0 \quad \text{for} \quad x < 0. \end{aligned} \quad (\text{A3.4.25})$$

Obviously,

$$\partial_x \Theta(x) = 0 \quad \text{for} \quad x \neq 0; \quad (\text{A3.4.26})$$

integrating $\partial_x \Theta(x)$ on the range $-\Delta x < x < \Delta x$, we find that

$$\int_{-\Delta x}^{\Delta x} dx \partial_x \Theta(x) = \Theta(\Delta x) - \Theta(-\Delta x) = 1. \quad (\text{A3.4.27})$$

Thus, $\partial_x \Theta(x)$ has the same behavior [Eqs. (A3.4.1) and (A3.4.2)] as the δ function; hence,

$$\partial_x \Theta(x) = \delta(x). \quad (\text{A3.4.28})$$

A3.4.5 Derivatives of $|x|$

Differentiating $|x|$, we find that

$$\begin{aligned} \partial_x |x| &= 1 & \text{for } x > 0, \\ \partial_x |x| &= -1 & \text{for } x < 0. \end{aligned} \quad (\text{A3.4.29})$$

$\partial_x |x|_{|x=0}$ is undefined because the derivative does not exist. One might be tempted to define it by

$$\partial_x |x|_{|x=0} = \frac{\partial_x |x|_{|x<0} + \partial_x |x|_{|x>0}}{2} = 0, \quad (\text{A3.4.30})$$

but this is inconsistent with that fact that

$$\frac{1 + \partial_x |x|}{2} = \Theta(x) \quad (\text{A3.4.31})$$

for all $x \neq 0$ (but arbitrarily close to 0). Since $\Theta(0) = 1$, it is logical to conclude that

$$\partial_x |x|_{|x=0} = 1. \quad (\text{A3.4.32})$$

Then, Eq. (A3.4.32) gives

$$(\partial_x |x|_{|x=0})^2 = 1. \quad (\text{A3.4.33})$$

This assignment is consistent with the fact that $(\partial_x |x|)^2 = 1$ for x arbitrarily close to 0. We thus conclude that

$$(\partial_x |x|)^2 = 1 \quad (\text{A3.4.34})$$

for all real x . Integrating the derivative of $\partial_x^2 |x|$ from $-L$ to $+L$, where $L > 0$, and taking the limit $L \rightarrow \infty$, we obtain

$$\begin{aligned}
\int_{-\infty}^{\infty} dx \frac{d^2}{dx^2} |x| &= \lim_{L \rightarrow \infty} \int_{-L}^L dx \frac{d^2}{dx^2} |x|, \\
&= \lim_{L \rightarrow \infty} \left(\frac{d}{dx} |L| - \frac{d}{dx} |-L| \right). \\
&= 2.
\end{aligned} \tag{A3.4.35}$$

Since $\partial_x^2 |x| = 0$ for $x \neq 0$, this expression satisfies the property given by Eq. (A3.4.1) of the δ function; and from Eq. (A3.4.35) we see that $\partial_x^2 |x|/2$ has the property given by Eq. (A3.4.2) of the δ function. Hence,

$$\partial_x^2 |x| = 2\delta(x). \tag{A3.4.36}$$

A3.4.6 sgn(x)

The function $\text{sgn}(x)$ is defined by

$$\begin{aligned}
\text{sgn}(x) &= 1 \quad \text{for } x > 0, \\
\text{sgn}(x) &= -1 \quad \text{for } x < 0.
\end{aligned} \tag{A3.4.37}$$

Although many authors write $\partial_x |x| = \text{sgn}(x)$, we do not because the often-used definition $\text{sgn}(0) = 0$ is inconsistent with Eq. (A3.4.32).

Appendix 3.5 Discrete Green's Function for the Finite Difference Model of the Damped Harmonic Oscillator

Just as an inhomogeneous differential equation can be solved in terms of a Green's function, an inhomogeneous difference equation can be solved in terms of what we call a discrete Green's function (DGF). In general, the DGF for a finite difference model of a differential equation is not simply a discretized version of the Green's function for the differential equation $g_{\tau-\tau'} \neq G(\tau \Delta t - \tau' \Delta t)$.

The solution of a difference equation such as

$$\psi_{\tau+1} - B\psi_{\tau} + C\psi_{\tau-1} = f_{\tau} \tag{A3.5.1}$$

with the initial conditions

$$\psi_{-1} = \psi_0 = 0 \tag{A3.5.2}$$

can be expressed in terms of a DGF, $g_{\tau-\tau'}$, of the form

$$\psi_\tau = \sum_{\tau'=0}^{\infty} f_{\tau'} g_{\tau-\tau'}, \quad (\text{A3.5.3})$$

where we take $f_\tau = 0$ and $\psi_\tau = 0$ for $\tau \leq 0$.

The appropriate DGF must satisfy both

$$g_{\tau+1-\tau'} - B g_{\tau-\tau'} + C g_{\tau-1-\tau'} = \delta_{\tau-\tau',0} \quad (\text{A3.5.4})$$

and the initial conditions. The Kronecker δ is defined by $\delta_{n,n'} = 1$ if $n = n'$ and $\delta_{n,n'} = 0$ if $n \neq n'$. Without loss of generality, we can choose $\tau' = 0$, so $\tau = \tau - \tau'$, and Eq. (A3.5.4) becomes

$$g_{\tau+1} - B g_\tau + C g_{\tau-1} = \delta_{\tau,0}. \quad (\text{A3.5.5})$$

This equation can be solved using the one-sided Z transform (see Note A3.5.1). Taking $g_{-1} = g_0 = 0$, the Z transform of Eq. (A3.5.5) is

$$(z^2 - Bz + C)\tilde{g}(z) = z, \quad (\text{A3.5.6})$$

where $\tilde{g}$ is the Z transform of g . Solving for $\tilde{g}$, we find that

$$\tilde{g}(z) = \frac{z}{z^2 - Bz + C}. \quad (\text{A3.5.7})$$

The denominator of Eq. (A3.5.7) can be expressed as the partial fraction expansion (see Note A3.5.2),

$$\frac{1}{(z - r_+)(z - r_-)} = \frac{1}{r_+ - r_-} \left(\frac{1}{z - r_+} - \frac{1}{z - r_-} \right), \quad (\text{A3.5.8})$$

where the $r_\pm$ are the roots of $z^2 - Bz + C = 0$, and

$$r_\pm = \frac{1}{2} \left(B \pm \sqrt{B^2 - 4C} \right). \quad (\text{A3.5.9})$$

Thus,

$$\tilde{g}(z) = \frac{1}{r_+ - r_-} \left(\frac{z}{z - r_+} - \frac{z}{z - r_-} \right). \quad (\text{A3.5.10})$$

Taking the inverse Z transform Z^{-1} of Eq. (A3.5.7), we find that

$$g_\tau = \Theta(\tau) \frac{r_+^\tau - r_-^\tau}{r_+ - r_-}, \quad (\text{A3.5.11})$$

where the step function enforces the condition $g_{\tau \leq 0} = 0$. The solution of Eq. (A3.5.1) is thus

$$\psi_\tau = \frac{1}{r_+ - r_-} \sum_{\tau'=0}^{\tau-1} f_{\tau'} \left(r_+^{\tau-\tau'} - r_-^{\tau-\tau'} \right). \quad (\text{A3.5.12})$$

Because of the step function in Eq. (A3.5.11), the summation needs to be carried out only to $\tau - 1$ instead of to ∞ .

Note A3.5.1:

The Z transform

The one-sided Z transform is defined by $Z[f_\tau] = \tilde{f}(z)$, where

$$\tilde{f}(z) = \sum_{\tau=0}^{\infty} f_\tau z^{-\tau}. \quad (\text{A3.5.13})$$

Directly from the definition, it can be shown that

$$Z(f_{\tau+1}) = z\tilde{f}(z) - f_0, \quad (\text{A3.5.14})$$

$$Z(f_{\tau-1}) = z^{-1}\tilde{f}(z), \quad (\text{A3.5.15})$$

$$Z(\delta_{\tau,0}) = 1. \quad (\text{A3.5.16})$$

The inverse Z transform Z^{-1} of

$$\tilde{f}(z) = \frac{z}{z-a} \quad (\text{A3.5.17})$$

can be found by noting that

$$\frac{z}{z-a} = \frac{1}{1-a/z} = 1 + a/z + (a/z)^2 + \cdots = \sum_{\tau=0}^{\infty} \left(\frac{a}{z}\right)^\tau, \quad (\text{A3.5.18})$$

assuming that $|a/z| < 1$. Thus, directly from the definition, we see that

$$Z(a^\tau) = \frac{a}{z-a}; \quad (\text{A3.5.19})$$

hence,

$$Z^{-1}\left(\frac{a}{z-a}\right) = a^\tau. \quad (\text{A3.5.20})$$

Note A3.5.2:**Partial fraction expansion**

Let

$$\frac{1}{(x-a)(x-b)} = \frac{\alpha}{(x-a)} + \frac{\beta}{(x-b)}, \quad (\text{A3.5.21})$$

which implies that

$$1 = \alpha(x-b) + \beta(x-a). \quad (\text{A3.5.22})$$

Let us assume Eq. (A3.5.21) to be an identity that is valid for all x ; thus, for $x = a$ and $x = b$, we find that $\alpha = 1/(a-b)$, $\beta = -\alpha$; hence,

$$\frac{1}{(x-a)(x-b)} = \frac{1}{a-b} \left[\frac{1}{(x-a)} - \frac{1}{(x-b)} \right]. \quad (\text{A3.5.23})$$

References

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Chapter 4

The 1D Wave Equation

In a uniform medium, Maxwell's equations reduce to the wave equation, and analytic solutions are derived by solving the wave equation subject to the appropriate boundary conditions. Although the 1D wave equation may seem simple, when boundary and initial conditions are specified and when sources are included, its analytical solutions are far from trivial and sometimes do not even exist.

Before moving on to FDTD for the wave equation, we develop some analytical solutions to which numerical solutions can be compared.

Topics:

- Derivation and various forms of wave equation
- Analytical solutions
- Extra topics: relativity from the wave equation
- Green's function and associated mathematics

4.1 The Homogeneous Wave Equation

4.1.1 General solution in an unbounded uniform medium

The simplest form of the wave equation (see Appendix 4.1 for a derivation) is

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = 0, \quad (4.1)$$

where v is the phase velocity. If no initial and boundary conditions are specified, it can be verified by direct substitution that the general solution is

$$\psi(x, t) = f(x - vt) + g(x + vt), \quad (4.2)$$

where f and g are arbitrary functions.

Letting $\psi(x, t) = f(x - vt)$,

$$\begin{aligned}\psi(x + \Delta x, t + \Delta t) &= f[x + v\Delta t - v(t + \Delta t)] \\ &= f[x - vt + (\Delta x - v\Delta t)].\end{aligned}\quad (4.3)$$

If $\Delta x = v\Delta t$, then $\psi(x + \Delta x, t + \Delta t) = \psi(x, t)$, and the shape of the disturbance described by f is the same at space–time points (x, t) and $(x + v\Delta t, t + \Delta t)$; hence, the disturbance moves with velocity v in the $+x$ direction.

Similarly, $g(x + vt)$ describes a disturbance traveling in the $-x$ direction with velocity v . Thus, in Eq. (4.1), v is the velocity (technically the phase velocity) of the wave. It is often mathematically convenient to use another solution obtained by putting $f(x) \rightarrow f(-x)$ so that

$$\psi(x, t) = f(vt \mp x) \quad (4.4)$$

describes a wave moving in the $\pm x$ direction.

4.1.2 Monochromatic solutions

Monochromatic solutions are infinite waves of the form

$$\psi(x, t) = e^{i(kx \mp \omega t)} \quad (4.5a)$$

$$= \sin(kx \mp \omega t) \quad (4.5b)$$

$$= \cos(kx \mp \omega t). \quad (4.5c)$$

By direct substitution, it can be verified that these functions are solutions to the wave equation if

$$\omega = vk, \quad (4.6)$$

where ω is the angular frequency, k is the wavenumber, $T = 2\pi/\omega$ is the period, and $\lambda = 2\pi/k$ is the wavelength. An alternative formulation is

$$\psi(x, t) = e^{i(\omega t \mp kx)} \quad (4.7a)$$

$$= \sin(\omega t \mp kx) \quad (4.7b)$$

$$= \cos(\omega t \mp kx). \quad (4.7c)$$

4.1.3 Reflecting cavity

When the wave vanishes on a boundary, for example, at the fixed ends of the string depicted in Fig. 4.1, solutions of the wave equation are much more complicated. For example, let

$$\psi(0, t) = 0, \quad (4.8a)$$

$$\psi(a, t) = 0. \quad (4.8b)$$

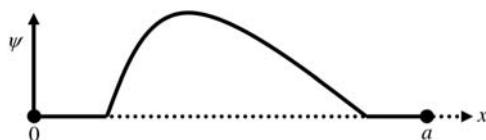


Figure 4.1 String fixed at two endpoints.

Now the functions f and g in Eq. (4.2) are no longer arbitrary. Using what is called *separation of variables*, we postulate a solution of the form $\psi(x, t) = X(x)T(t)$ and insert it into the wave equation to obtain

$$\frac{T''(t)}{T(t)} = v^2 \frac{X''(x)}{X(x)}. \quad (4.9)$$

Since X and T are independent of each other and are functions of different independent variables, Eq. (4.9) holds for all x and t only if both sides equal the same constant, call it $-\omega^2$, $\omega^2 > 0$ (see Note 4.1). Thus,

$$\frac{T''(t)}{T(t)} = -\omega^2, \quad (4.10)$$

$$\frac{X''(x)}{X(x)} = -k^2, \quad (4.11)$$

where

$$k = \omega/v. \quad (4.12)$$

Note 4.1

In Eq. (4.10) we could have chosen $T''(t)/T(t) = +\omega^2$ instead of $-\omega^2$, but this yields the non-oscillating solutions $T(t) = e^{\omega t}$, $\sinh(\omega t)$, $\cosh(\omega t)$, and $X(x) = e^{kx}$, $\sinh(kx)$, $\cosh(kx)$, which cannot satisfy the boundary and initial conditions. The lesson here is that problems cannot be solved by mathematics alone, without physical insight.

Solutions of Eq. (4.10) are $T(t) = \cos(\omega t)$, $\sin(\omega t)$, and $e^{\pm \omega t}$, and the most general real-valued solution is

$$T(t) = A\cos(\omega t) + B\sin(\omega t), \quad (4.13)$$

where A and B are arbitrary constants. Similarly, the most general solution of Eq. (4.11) is

$$X(x) = C\cos(kx) + D\sin(kx). \quad (4.14)$$

The boundary conditions given by Eq. (4.8) can be satisfied at all t by requiring that

$$X(0) = 0, \quad (4.15a)$$

$$X(a) = 0. \quad (4.15b)$$

Since $X(0) = 0$, which implies that $C = 0$, in Eq. (4.14), $X(x) = D\sin(kx)$. To satisfy Eq. (4.15), we require that $k = k_n$, where

$$k_n = \frac{n\pi}{a}, \quad (4.16)$$

where $n = 1, 2, 3, \dots$. Thus, $X = X_n$, where

$$X_n(x) = \sin(k_n x). \quad (4.17)$$

Because of Eq. (4.12), once the k_n values are fixed, the values of ω are restricted to $\omega = \omega_n$, where

$$\omega_n = \nu k_n. \quad (4.18)$$

Because of the boundaries, there are only solutions—called *eigenfunctions*—of certain discrete frequencies (*eigenfrequencies*).

Thus, the most general solution of the wave equation together with the boundary conditions of Eq. (4.8) is a Fourier sum given by

$$\psi(x, t) = \sum_{n=1}^{\infty} [c_n \sin(\omega_n t) + d_n \cos(\omega_n t)] \sin(k_n x), \quad (4.19)$$

where $\omega_n = \nu k_n$; and c_n and d_n are arbitrary constants.

With reference to Fig. 4.1, let the shape of the string at $t = 0$ be

$$\psi(x, 0) = f(x), \quad (4.20)$$

where $f(0) = f(a) = 0$. Let the string be released from rest so that

$$\partial_t \psi(x, t)|_{t=0} = 0. \quad (4.21)$$

The solution given in Eq. (4.19) can be made to satisfy the initial condition [Eq. (4.21)] by choosing $c_n = 0$ for all n . Finally, Eq. (4.19) can be made to satisfy Eq. (4.20) by setting

$$d_n = \frac{2}{a} \int_0^a dx f(x) \sin(k_n x). \quad (4.22)$$

For example, if $\psi(x, 0) = \sin(k_1 x)$, then $d_1 = 1$, and $d_{n \neq 1} = 0$, so the solution becomes

$$\psi(x, t) = \cos(\omega_1 t) \sin(k_1 x). \quad (4.23)$$

4.1.4 Boundary conditions at medium interfaces

We often want to solve problems in which waves propagate in different media. The simplest case is that of piecewise uniform media (continuously variable ones can be approximated by thin slices of piecewise uniform media).

Let two different media meet at $x = 0$, and let $\nu = \nu_1$ for $x < 0$ and $\nu = \nu_2$ for $x \geq 0$. To the left ($x \leq 0$) of the interface, the solution of the wave equation is ψ_1 , and to the right ($x > 0$) of the interface, it is ψ_2 . Since the string does not break, ψ must be a continuous function across the interface, which implies the boundary condition

$$\psi_1(0, t) = \psi_2(0, t). \quad (4.24a)$$

The wave equation tells us that the up-down acceleration of the string is $\partial_t^2 \psi = \nu^2 \partial_x^2 \psi$. Since any physically realizable acceleration must be finite, $\partial_x^2 \psi$ must also be finite. For $\partial_x^2 \psi$ to be finite, $\partial_x \psi$ must be continuous; thus, at the interface,

$$\partial_x \psi_1(x, t)|_{x=0} = \partial_x \psi_2(x, t)|_{x=0}. \quad (4.24b)$$

Returning to the string model of Appendix 4.1, where strings of different densities meet, the tension in the string must be the same across the boundary in equilibrium (where $\psi = 0$); otherwise, the point at the interface would accelerate to the left or right. Since displacements from equilibrium are assumed to be small, it is an excellent approximation to regard the tension T as constant across the boundary so that $v_1^2 = T/\rho_1$ and $v_2^2 = T/\rho_2$ (where $\rho = \rho_1$ for $x < 0$ and $\rho = \rho_2$ for $x \geq 0$). Let ν_0 be a constant and let $\nu = \nu_0/n$, where $n = \sqrt{\rho}$ is called the index of refraction; thus, $n_{1,2} = \sqrt{\rho_{1,2}}$.

When a monochromatic wave encounters an interface between two media, its frequency is unaffected; thus, $\omega = v_1 k_1 = v_2 k_2$, which implies that $k_1/n_1 = k_2/n_2$. Therefore, $k_2 = (n_2/n_1)k_1$ or $k_2 = nk_1$, where $n = n_2/n_1$ is the refractive index of medium 2 relative to medium 1.

Now letting density be a function of position, i.e., $n(x) = \sqrt{\rho(x)}$, it follows that $\nu(x) = \nu_0/n(x)$, and the wave equation becomes

$$\left(\partial_t^2 - \frac{\nu_0^2}{n^2} \partial_x^2 \right) \psi(x, t) = 0, \quad (4.25)$$

where

$$k(x) = n(x) k_0, \quad (4.26)$$

and $k_0 = \omega/\nu_0$. Although the wavelength changes across the interface, the frequency does not (according to physical reasoning, not mathematics).

4.1.5 Reflection and transmission at a medium interface

Figure 4.2 depicts an interface between two different media for which

$$n = n_1 \quad \text{for } x < 0, \quad (4.27a)$$

$$n = n_2 \quad \text{for } x \geq 0. \quad (4.27b)$$

Let a wave traveling in the $+x$ direction, $\psi_i(x, t) = f[k_1(v_1 t - x)]$, impinge on the interface. From physical considerations, we know that the wave is partially reflected and partially transmitted. Let the reflected wave be given by $\psi_r(x, t) = rf[k_1(v_1 t + x)]$, where r is the reflection coefficient. Thus, for $x < 0$, the wave function is

$$\begin{aligned} \psi_1(x, t) &= f[k_1(v_1 t - x)] + rf[k_1(v_1 t + x)] \\ &= f(\omega t - k_1 x) + rf(\omega t + k_1 x). \end{aligned} \quad (4.28)$$

Similarly, for $x \geq 0$, the transmitted wave is

$$\begin{aligned} \psi_2(x, t) &= \tau f[k_2(v_2 t - x)] \\ &= \tau f(\omega t - k_2 x), \end{aligned} \quad (4.29)$$

where τ is the transmission coefficient.

The boundary conditions given by Eq. (4.24) now yield

$$f(\omega t) + rf(\omega t) = \tau f(\omega t), \quad (4.30a)$$

$$-k_1 f'(\omega t) + rk_1 f'(\omega t) = -\tau k_2 f'(\omega t). \quad (4.30b)$$

Solving for r and τ , we find that

$$r = \frac{(n_1/n_0) - 1}{(n_1/n_0) + 1}, \quad (4.31)$$

$$\tau = \frac{2}{(n_1/n_0) + 1}. \quad (4.32)$$

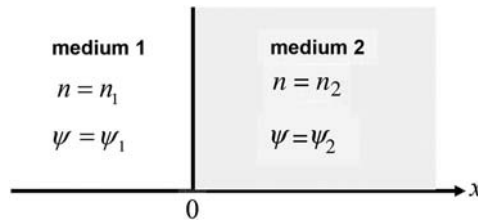


Figure 4.2 Interface between two media.

If $n_1/n_0 = 1$, there is no reflection, and the wave is completely transmitted through the interface. In the limit $n_1/n_0 \rightarrow \infty$, $r \rightarrow -1$, and $\tau \rightarrow 0$. In this case, the wave is completely reflected, but its phase changes by π .

When a wave is incident from a high-refractive-index material to one with a lower refractive index ($n_2 < n_1$), $n_1/n_0 < 1$, but Eqs. (4.31) and (4.32) still hold.

4.1.6 Reflection and transmission of a layer

A case of great interest is the single layer (Fig. 4.3). Taking $n = 1$ in the $x < 0$ region, $n = n_s$ in the $0 \leq x < a$ region, and $n = 1$ for $x \geq a$; applying the boundary conditions given by Eq. (4.24), it is shown in Appendix 4.3 that

$$r = \frac{i(n_s^2 - 1)\sin(n_s k_0 a)}{2n_s \cos(n_s k_0 a) - i(n_s^2 + 1)\sin(n_s k_0 a)}, \quad (4.33)$$

$$\tau = \frac{2n_s e^{-ik_0 a}}{2n_s \cos(n_s k_0 a) - i(n_s^2 + 1)\sin(n_s k_0 a)}. \quad (4.34)$$

Antireflection layer

If $n_s k_0 a = m\pi$ (m is an integer), then from Eqs. (4.33) and (4.34) it is easy to see that $r = 0$ and $\tau = 1$. Thus, an incident wave of wavenumber k_0 is totally transmitted (with no reflection). Antireflection coatings (for lenses) can be fabricated by combining layers of different thicknesses and refractive indices. Of course, in three dimensions at arbitrary incidence angles, it is more complicated.

The interior field ($0 < x < a$) is

$$\psi_{01}(x, t) = e^{i\omega t} (a_{01}^+ e^{-ik_{01} x} + a_{01}^- e^{ik_{01} x}), \quad (4.35)$$

where $k_{01} = n_s k_0$, and

$$a_{01}^\pm = \left(\frac{n_s \pm 1}{2n_s} \right) + \left(\frac{n_s \mp 1}{2n_s} \right) r. \quad (4.36)$$

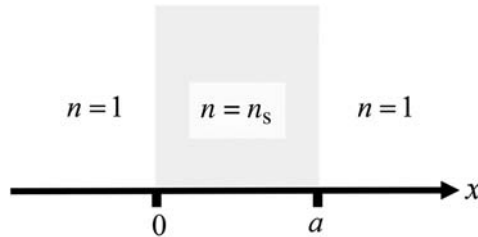


Figure 4.3 Layer of width a and refractive index n_s relative to the ambient medium.

The reflected and transmitted intensities are $R = |r|^2$ and $T = |\tau|^2$, respectively, where

$$R = \frac{(n_s^2 - 1)^2 \sin^2(n_s k_0 a)}{(n_s^2 - 1)^2 \sin^2(n_s k_0 a) + 4n_s^2}, \quad (4.37)$$

$$T = \frac{4n_s^2}{(n_s^2 - 1)^2 \sin^2(n_s k_0 a) + 4n_s^2}. \quad (4.38)$$

4.2 The Damped Wave Equation

In one dimension, the damped (absorbing or lossy) wave equation is

$$\left(\partial_t^2 + 2\alpha \partial_t - \frac{v^2}{n^2} \partial_x^2 \right) \psi(x, t) = 0, \quad (4.39)$$

where n is the refractive index, and $\alpha > 0$ is the absorption. The customary factor of 2 simplifies the algebra that follows.

The inclusion of a loss term complicates the solution. There is no general solution in the form of Eq. (4.2), and there are two quite different solutions.

Solution 1: complex frequency

Postulating a solution of the form $\psi(x, t) = e^{i(\omega t - n k x)}$ and substituting into Eq. (4.39) gives

$$-w^2 + 2i\alpha w + v^2 k^2 = 0. \quad (4.40)$$

Solving for w , we find that

$$w = i\alpha \pm \omega', \quad (4.41)$$

where

$$\omega = v k, \quad (4.42)$$

and

$$\omega' = \sqrt{\omega^2 - \alpha^2}. \quad (4.43)$$

Forward/backward ($\pm x$ directions)-moving solutions are thus

$$\psi_{\pm}(x, t) = e^{-\alpha t} e^{i(\pm \omega' t - n k x)}. \quad (4.44)$$

To ensure that the solution is a decaying oscillation, we impose the condition

$$0 \leq \alpha < \omega. \quad (4.45)$$

Comparing solution Eq. (4.44) with that of the damped harmonic oscillator (Section 3.5.1), we see that the time dependence is the same.

The loss term gives rise to dispersive effects—different frequencies have different velocities and different rates of attenuation. For angular frequency component $\omega = 2\pi/T$, the amplitude falls by a factor of $e^{-\alpha T}$ for each wave period.

Solution 2: complex wavenumber and complex refractive index

Another solution can be derived by postulating a solution of the form

$$\psi(x, t) = e^{i(\omega t \mp k' x)}, \quad (4.46)$$

where k' is complex. Substituting Eq. (4.46) into Eq. (4.39) and solving for k' gives

$$\begin{aligned} k'^2 &= \frac{n^2}{v^2} (\omega^2 - 2i\alpha\omega) \\ &= k^2 n^2 \left(1 - \frac{2i\alpha}{\omega} \right). \end{aligned} \quad (4.47)$$

Defining the complex refractive index to be $n_c = k'/k$, we find that

$$n_c = n \left(1 - \frac{2i\alpha}{\omega} \right)^{1/2}. \quad (4.48)$$

Some rather tedious but straightforward algebra gives

$$\begin{aligned} \sqrt{1 - 2i\alpha/\omega} &= \frac{1}{\sqrt{2\omega}} \left[(\sqrt{\omega^2 + 4\alpha^2} + \omega)^{1/2} - i(\sqrt{\omega^2 + 4\alpha^2} - \omega)^{1/2} \right]; \text{ hence,} \\ k' &= \frac{nk}{\sqrt{2\omega}} \left[(\sqrt{\omega^2 + 4\alpha^2} + \omega)^{1/2} - i(\sqrt{\omega^2 + 4\alpha^2} - \omega)^{1/2} \right]. \end{aligned} \quad (4.49)$$

For $\alpha/\omega \ll 1$,

$$\frac{n_c}{n} \cong 1 + \frac{\alpha^2}{2\omega^2} - i\frac{\alpha}{\omega}. \quad (4.50)$$

The damped wave equation [Eq. (4.39)] can be formally expressed in terms of the complex refractive index as

$$\left(\partial_t^2 - \frac{v^2}{n_c^2} \partial_x^2 \right) \psi(x, t) = 0. \quad (4.51)$$

Note 4.2

This is a useful heuristic form, but the solutions of Eq. (4.51) differ from those of Eq. (4.39) when a source is included.

Forward/backward-moving solutions are thus

$$\psi_{\pm}(x, t) = e^{i(\omega t \mp n_c k x)}. \quad (4.52)$$

Mathematically, both Eqs. (4.44) and (4.52) are valid solutions to the damped wave equation, but their behavior is quite different. Which one is appropriate depends on the problem to be solved. If an initial field is specified in an absorbing medium, then the complex frequency solution tells us that it decreases with time as $e^{-\alpha t}$ at every point in space. However, this is a rather rare case. When a wave propagates from a lossless medium into an absorbing one, it attenuates with distance into the absorbing medium, and thus the complex wavenumber solution is appropriate. In Appendix 4.3, where we consider propagation through layered structures, the complex-wavenumber solution is used. The frequency is the same in all of the layers, and the analysis holds for complex wavenumber and complex refractive index.

If the wave is generated by a source in an absorbing medium, then it attenuates as it propagates outward from the source, so again the complex-wavenumber form is the correct solution.

The complex-wavenumber solution is also intrinsically dispersive. Short-wavelength (high-frequency) components attenuate faster than long-wavelength (low-frequency) components, and thus the latter travel further. Animals such as elephants exploit this effect to communicate over long distances with low-frequency sound.

4.3 Wave Equations with a Source in Unbounded Space

4.3.1 Lossless wave equation

The wave equation with a source is

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = s(x, t), \quad (4.53)$$

where s is a source. The solution is given in terms of the Green's function G (see Appendix 4.4) by

$$\psi(x, t) = \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dx' G(x - x', t - t') s(x', t'), \quad (4.54)$$

where G satisfies the initial and boundary conditions of ψ .

Let s switch on at time $t = 0$ such that

$$s(x, t) = 0 \quad \text{for} \quad t \leq 0 \quad (4.55)$$

and assume that before the source turns on there is no field. Thus, the initial conditions are

$$\psi(x, t) = 0 \quad \text{for } t \leq 0, \quad (4.56a)$$

$$\partial_t \psi(x, t) = 0 \quad \text{for } t \leq 0. \quad (4.56b)$$

As shown in Appendix 4.4, the appropriate Green's function is

$$G(x - x', t - t') = \frac{1}{2v} \Theta[v(t - t') - |x - x'|], \quad (4.57)$$

where Θ is the step function defined by $\Theta(t) = 0$ for $t < 0$ and $\Theta(t) = 1$ for $t \geq 0$ (see Appendix 3.4).

Harmonic point source turned on instantaneously at time = 0

Taking $s(x, t) = \Theta(t)\delta(x)e^{i\omega t}$ and carrying out the integration in Eq. (4.54), we obtain the solution $\psi = \psi_0$, where

$$\psi_0(x, t) = \frac{1}{2i v^2 k} \Theta(vt - |x|) [e^{i(\omega t - k|x|)} - 1], \quad (4.58)$$

and $v = \omega/k$.

It can be verified that

$$\Theta(vt - |x|) = \Theta(t) \Theta(vt - |x|) \quad (4.59)$$

because $|x| \geq 0$. Using Eq. (4.59), it is interesting to verify that ψ_0 is the solution of

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = \Theta(t) \delta(x) e^{i\omega t}. \quad (4.60)$$

Substituting ψ_0 into Eq. (4.60) and using the properties of the step function and the derivatives of $|x|$ (see Appendix 3.4), we find that

$$(\partial_t^2 - v^2 \partial_x^2) \psi_0(x, t) = \Theta(vt - |x|) \delta(x) e^{i(\omega t - k|x|)} + \frac{1}{ikv} [e^{i(\omega t - k|x|)} - 1] \delta(x) \delta(t). \quad (4.61)$$

It is easy to see that

$$\delta(x) \Theta(vt - |x|) e^{i(\omega t - k|x|)} = \delta(x) \Theta(t) e^{i\omega t} \quad (4.62)$$

because $v > 0$, and at $x = 0$, $\Theta(vt - |x|) = \Theta(t)$ and $e^{i(\omega t - k|x|)} = e^{i\omega t}$. Since $e^{i(\omega t - k|x|)} - 1 = 0$ at $t = 0$, and $\delta(t) = 0$ for $t \neq 0$, we conclude that

$$[e^{i(\omega t - k|x|)} - 1] \delta(x) \delta(t) = 0, \quad (4.63)$$

and thus verify that ψ_0 is indeed the solution of Eq. (4.60).

Note 4.3

This kind of reasoning might seem strange and unnatural, but it is unavoidable because the δ function is not an ordinary function, but a *distribution*. See Appendix 3.4.

The real and imaginary parts of ψ_0 , $\psi_{\text{Re}0} = \text{Re}(\psi_0)$, and $\psi_{\text{Im}0} = \text{Im}(\psi_0)$, given by

$$\psi_{\text{Re}0}(x, t) = \frac{1}{2v^2k} \Theta(\omega t - k|x|) \sin(t - |x|/v), \quad (4.64)$$

and

$$\psi_{\text{Im}0}(x, t) = \frac{1}{2v^2k} \Theta(\omega t - k|x|) [1 - \cos(t - |x|/v)], \quad (4.65)$$

respectively, are solutions of

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = \delta(x) \Theta(t) \cos(\omega t), \quad (4.66)$$

and

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = \delta(x) \Theta(t) \sin(\omega t), \quad (4.67)$$

respectively.

Devil in the details

As noted in Appendix 4.4, there are two more functions,

$$G_1 = \frac{v}{2} \Theta(t - |x|/v), \quad (4.68)$$

and

$$G_2 = \frac{1}{2k\omega} \Theta(\omega t - k|x|), \quad (4.69)$$

that satisfy

$$(\partial_t^2 - v^2 \partial_x^2) G(x, t) = \delta(x) \delta(t), \quad (4.70)$$

but putting these Green's functions into the integration of Eq. (4.54) does not yield the correct solution [Eq. (4.58)]. For example,

$$\begin{aligned} \psi_1(x, t) &= \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dx' G_1(x - x', t - t') \Theta(t') \delta(x') e^{i\omega t'} \\ &= \frac{1}{2ik} \Theta(t - |x|/v) [e^{i(vk t - k|x|)} - 1]. \end{aligned} \quad (4.71)$$

It can be shown that $(\partial_t^2 - v^2 \partial_x^2) \psi_1(x, t) = v^2 \Theta(t) \delta(x) e^{i\omega t}$, and we see that Eq. (4.58) can be expressed in the alternative form

$$\psi_0(x, t) = \frac{1}{2i k v^2} \Theta(t - |x|/v) [e^{i(v k t - k|x|)} - 1]. \quad (4.72)$$

Although $\Theta(vt - |x|)$, $\Theta(t - |x|/v)$, and $\Theta(\omega t - k|x|)$ are all numerically equivalent, they are not quite equivalent in analytical calculations.

Harmonic point source turned on slowly at time = 0

FDTD calculations can be affected by transients that give rise to large errors. For future reference, when comparing analytic with FDTD solutions we find the field produced by a harmonic point source that is slowly turned on by an exponential or Gaussian turn-on function, such as

$$\Theta_e(t) = \Theta(t)(1 - e^{-\beta t}), \quad (4.73a)$$

$$\Theta_g(t) = \Theta(t)(1 - e^{-\beta^2 t^2}), \quad (4.73b)$$

respectively, where $\beta > 0$. In FDTD calculations, Θ_g is often used to turn on the sources, but for analytical simplicity we use Θ_e here. Taking $s(x, t) = \Theta_e(t) e^{i\omega t} \delta(x)$, the solution of

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = \Theta(t)(1 - e^{-\beta t}) e^{i\omega t} \delta(x) \quad (4.74)$$

is

$$\psi_e(x, t) = \psi_0(x, t) - \Delta\psi_e(x, t), \quad (4.75)$$

where $\Delta\psi_e(x, t)$ is the part of the solution due to the turn-on function. $\Delta\psi_e(x, t)$ satisfies

$$(\partial_t^2 - v^2 \partial_x^2) \Delta\psi_e(x, t) = \delta(x) \Theta(t) e^{i(\omega + i\beta)t}, \quad (4.76)$$

while ψ_0 is given by Eq. (4.58). We find that

$$\Delta\psi_e(x, t) = \frac{1}{2i \bar{\omega} v} \Theta(\omega t - k|x|) [e^{i(\bar{\omega} t - \bar{k}|x|)} - 1], \quad (4.77)$$

where $\bar{\omega} = \omega + i\beta$, and $\bar{k} = \bar{\omega}/v$.

4.3.2 Damped wave equation

The damped wave equation with a source is

$$(\partial_t^2 + 2\alpha \partial_t - v^2 \partial_x^2) \psi(x, t) = s(x, t). \quad (4.78)$$

The Green's function for the damped wave equation is much more difficult to find, so we use a more direct method to solve Eq. (4.78).

Harmonic point source turned on instantaneously at time = 0

Setting $s(x, t) = \delta(x)\Theta(t)e^{i\omega t}$, we seek the solution of

$$(\partial_t^2 + 2\alpha \partial_t - v^2 \partial_x^2)\psi(x, t) = \delta(x) \Theta(t) e^{i\omega t}. \quad (4.79)$$

Since the wave propagates symmetrically outward from the source, we postulate a solution of the form

$$\psi(x, t) = c \Theta(vt - |x|) e^{i(\omega t - k'|x|)}, \quad (4.80)$$

where c is a constant to be determined. Now putting Eq. (4.80) into Eq. (4.79), we find that

$$\begin{aligned} \partial_x^2 e^{-ik'|x|} &= -[k'^2(\partial_x|x|)^2 + ik'\partial_x^2|x|]e^{-ik'|x|} \\ &= -[k'^2 + 2ik'\delta(x)]e^{-ik'|x|}, \end{aligned} \quad (4.81)$$

where we have used $(\partial_x|x|)^2 = 1$ and $\partial_x^2|x| = 2\delta(x)$ (see Appendix 3.4). Requiring that $-\omega^2 + 2i\alpha\omega + k'^2v^2 = 0$ and defining $\omega = kv$, we find that

$$k' = k\sqrt{1 - 2i\alpha/\omega}. \quad (4.82)$$

Thus,

$$\begin{aligned} (\partial_t^2 + 2\alpha \partial_t - v^2 \partial_x^2)c[\Theta(vt - |x|)e^{i(\omega t - k'|x|)}] &= 2c\{ik'v^2\Theta(vt - |x|)\delta(x) \\ &+ v\delta(x)\delta(t) + [iv^2(k - k') + \alpha v]\delta(vt - |x|)\}e^{i(\omega t - k'|x|)}. \end{aligned} \quad (4.83)$$

Note that $\delta(vt - |x|)$ vanishes unless $|x| = vt$, so $\delta(vt - |x|)e^{i(\omega t - k'|x|)} = \delta(vt - |x|)e^{i(k - k')|x|}$ because $v = \omega/k$. Now, using Eq. (4.62), Eq. (4.83) becomes

$$\begin{aligned} (\partial_t^2 + 2\alpha \partial_t - v^2 \partial_x^2)c\Theta(vt - |x|) e^{i(\omega t - k'|x|)} \\ = 2ik'v^2c \Theta(vt - |x|)\delta(x)e^{i\omega t} + 2cv[i v(k - k') + \alpha]\delta(vt - |x|)e^{i(k - k')|x|} \\ + 2cv\delta(x)\delta(t)e^{i(\omega t - k'|x|)}. \end{aligned} \quad (4.84)$$

We drop the last two terms on the right of Eq. (4.84) because $\delta(x)\delta(t)$ vanishes everywhere except at $(x = 0, t = 0)$, and $\delta(vt - |x|)$ vanishes everywhere except at the leading edge of the wavefront beyond which the field vanishes. Requiring that $2ik'v^2c = 1$, we find that

$$c = \frac{1}{2i v^2 k'}, \quad (4.85)$$

and a solution of the damped wave equation with a source Eq. (4.79) is thus

$$\psi_0(x, t) = \frac{1}{2i v^2 k'} \Theta(vt - |x|) e^{i(\omega t - k'|x|)}. \quad (4.86)$$

Solution Eq. (4.86) does not rigorously satisfy the initial conditions of $\psi_0(x, 0) = \partial_t \psi_0(x, 0)$, but it does in a practical sense because at $t = 0$, $\Theta(vt - |x|) = \Theta(-|x|) = 0$ for any arbitrarily small value of $|x| \neq 0$; similarly, $\partial_t \psi_0(x, t)|_{t=0} = 0$ for all $|x| \neq 0$.

Note 4.4

Because k' is complex, $\Theta(vt - |x|)[e^{i(\omega t - k'|x|)} - 1]$ is not a solution of Eq. (4.79) and does not satisfy the initial conditions [Eq. (4.56)].

It is interesting to compare the complex-wavenumber solution [Eq. (4.86)] with the complex-frequency solution, which is found by postulating a solution of the form

$$\psi_{\text{cf}}(x, t) = c e^{i[(\omega' + i\alpha)t - k|x|]}. \quad (4.87)$$

In this case,

$$\psi_{\text{cf}}(x, t) = \frac{1}{2i v^2 k} \Theta(vt - |x|) [e^{-\alpha t} e^{i(\omega' t - k|x|)} - 1], \quad (4.88)$$

where $\omega'^2 = \omega^2 - \alpha^2$. The amplitude of ψ_{cf} decreases with time, but unlike the complex-wavenumber solution, it (counterintuitively) does not decrease with distance from the source. As we shall see in the next section, the FDTD solutions of the damped wave equation yield the complex-wavenumber solution, but not the complex-frequency solution.

Harmonic point source turned on slowly at time = 0

When a source turn-on function is included (as we saw for the lossless wave equation), the solution consists of two parts in the form of Eq. (4.75). In this case, ψ_0 is given by Eq. (4.86), and the total field $\psi_e = \psi_0 + \Delta\psi_e$ is the solution of

$$\begin{aligned} (\partial_t^2 + 2\alpha \partial_t - v^2 \partial_x^2) \psi_e(x, t) &= \delta(x) e^{i\omega t} (1 - e^{-\beta t}) \\ &= \delta(x) [e^{i\omega t} - e^{i(\omega + i\beta)t}], \end{aligned} \quad (4.89)$$

while $\Delta\psi_e(x, t)$ satisfies

$$(\partial_t^2 + 2\alpha \partial_t - v^2 \partial_x^2) \Delta\psi_e(x, t) = \delta(x) \Theta(t) e^{i(\omega+i\beta)t}. \quad (4.90)$$

Postulating the solution to be

$$\Delta\psi_e(x, t) = c e^{-ik''|x|} e^{i(\omega+i\beta)t}, \quad (4.91)$$

where k'' and c are to be determined, we find that

$$v^2 k''^2 = (\omega + i\beta)^2 - 2i\alpha(\omega + i\beta), \quad (4.92)$$

$$c = \frac{1}{2i v^2 k''}, \quad (4.93)$$

and thus,

$$\Delta\psi_e(x, t) = \frac{1}{2i v^2 k''} \Theta(vt - |x|) e^{-ik''|x|} e^{i(\omega+i\beta)t}. \quad (4.94)$$

4.4 Source in a Reflecting Cavity

In a reflecting cavity ($0 \leq x \leq a$), the wave equation

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = s(x, t) \quad (4.95)$$

has the boundary conditions

$$\psi(0, t) = 0, \quad (4.96a)$$

$$\psi(a, t) = 0. \quad (4.96b)$$

Again assuming that $s(x, t) = \psi(x, t) = 0$ for $t \leq 0$, the initial conditions are

$$\psi(x, t) = 0 \quad \text{for } t \leq 0, \quad (4.97a)$$

$$\partial_t \psi(x, t) = 0 \quad \text{for } t \leq 0. \quad (4.97b)$$

The solution is given in terms of a Green's function G (see Appendix 4.4) by

$$\psi(x, t) = \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dx' G(x, t; x', t') s(x', t'), \quad (4.98)$$

where

$$G(x, x', t - t') = \Theta(t - t') \frac{2}{a} \sum_{n=1}^{\infty} \frac{1}{\omega_n} \sin[\omega_n(t - t')] \sin(k_n x') \sin(k_n x), \quad (4.99)$$

$$k_n = n\pi/a, \text{ and } \omega_n = vk_n.$$

4.4.1 Point source switched on instantaneously

Let us now compute the field ψ_0 due to a point source at the origin that turns on at $t = 0$:

$$s(x, t) = \delta(x) \Theta(t) e^{i\omega t}. \quad (4.100)$$

Evaluating Eq. (4.98), we find that

$$\begin{aligned} \psi_0(x, t) &= \int_0^t dt' \sum_{n=1}^{\infty} \left[\frac{1}{n} \sin(k_n x_0) \sin(k_n x) \sin[\omega_n(t - t')] e^{i\omega t'} \right] \\ &= \frac{2}{\pi v} \sum_{n=1}^{\infty} \left\{ \frac{1}{n} \sin(k_n x) \sin(k_n x_0) \left[\frac{\omega_n \cos(\omega_n t) + i \omega \sin(\omega_n t) - \omega_n e^{i\omega t}}{\omega^2 - \omega_n^2} \right] \right\}. \end{aligned} \quad (4.101)$$

The solutions for $s(x, t) = \delta(x)\Theta(t)\cos(\omega t)$ and $s(x, t) = \delta(x)\Theta(t)\sin(\omega t)$ are, respectively,

$$\begin{aligned} \psi_c(x, t) &= \text{Re}[\psi_0(x, t)] \\ &= \frac{2}{\pi v} \sum_{n=1}^{\infty} \left\{ \frac{1}{n} \sin(k_n x) \sin(k_n x_0) \omega_n \left[\frac{\cos(\omega_n t) - \cos(\omega t)}{\omega^2 - \omega_n^2} \right] \right\}, \end{aligned} \quad (4.102)$$

and

$$\begin{aligned} \psi_s(x, t) &= \text{Im}[\psi_0(x, t)] \\ &= \frac{2}{\pi v} \sum_{n=1}^{\infty} \left\{ \frac{1}{n} \sin(k_n x) \sin(k_n x_0) \left[\frac{\omega \sin(\omega_n t) - \omega_n \sin(\omega t)}{\omega^2 - \omega_n^2} \right] \right\}. \end{aligned} \quad (4.103)$$

It is interesting to examine the case where $\omega \rightarrow \omega_m$. For ψ_s , we find that

$$\lim_{\omega \rightarrow \omega_m} \left[\frac{\omega \sin(\omega_m t) - \omega_n \sin(\omega t)}{\omega^2 - \omega_m^2} \right] = \frac{1}{2} \left[\frac{\sin(\omega_m t)}{\omega_m} - t \cos(\omega_m t) \right]. \quad (4.104)$$

Thus, at $\omega = \omega_m$, ψ_s grows with t , except where $\sin(k_n x_0) \neq 0$. As $t \rightarrow \infty$, the m^{th} term in Eq. (4.102) dominates; thus, for large t ,

$$\psi_s(x, t) \rightarrow -\frac{\sin(k_m x_0)}{m\pi v} t \cos(\omega_m t) \sin(k_m x). \quad (4.105)$$

This is a resonance, in which the amplitude of a standing-wave mode continuously grows.

4.4.2 Point source switched on slowly

Now let the point source switch on slowly by taking $s(x, t) = \delta(x)\Theta_e(t)e^{i\omega t}$. This source generates the field $\psi_e = \psi_0 - \Delta\psi_e$, where $\Delta\psi_e$ satisfies

$$(\partial_t^2 - v^2 \partial_x^2)\psi(x, t) = \delta(x)\Theta(t)e^{-\beta t}e^{i\omega t}. \quad (4.106)$$

Evaluating Eq. (4.98) with this source, we find that

$$\Delta\psi_e(x, t) = \frac{2}{\pi v} \sum_{n=1}^{\infty} \left[\frac{1}{n} \sin(k_n x_0) \sin(k_n x) K_n(t) \right], \quad (4.107)$$

where

$$\begin{aligned} K_n(t) &= \int_0^t dt' e^{i(\omega + i\alpha)t'} \sin[\omega_n(t - t')] \\ &= \frac{\omega_n \cos(\omega_n t) + (i\omega - \alpha) \sin(\omega_n t) - \omega_n e^{i\omega t} e^{-\alpha t}}{(\omega + i\alpha)^2 - \omega_n^2}. \end{aligned} \quad (4.108)$$

4.5 The Scattered Field

In the scattering problem, a scatterer S is immersed in what we call the substrate, and a wave ψ_0 is incident upon it. Taking the index of refraction relative to the substrate to be n_s , the wave equation becomes

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \partial_x^2 \right) \psi(x, t) = 0, \quad (4.109)$$

where $n = n_s$, 1 inside and outside of the scatterer, respectively. The total wave field ψ can be decomposed into the sum of the incident field and the scattered field ψ_s :

$$\psi = \psi_0 + \psi_s. \quad (4.110)$$

The incident field propagates (by definition) as if there were no scatterer and thus obeys

$$(\partial_t^2 - v_0^2 \partial_x^2) \psi_0(x, t) = 0. \quad (4.111)$$

It is thus the scattered field that carries physical information about the scatterer. Subtracting Eq. (4.110) from Eq. (4.111), we obtain the wave equation for the scattered field,

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \partial_x^2 \right) \psi_s(x, t) = s_0(x, t), \quad (4.112)$$

where

$$\begin{aligned}
s_0(x, t) &= -\left(\frac{n^2-1}{n^2}\right) \partial_t^2 \psi_0(x, t) \\
&= -\left(\frac{n_s^2-1}{n_s^2}\right) \partial_t^2 \psi_0(x, t) && \text{for } x \in \mathbf{S} \\
&= 0 && \text{for } x \notin \mathbf{S},
\end{aligned} \tag{4.113}$$

and $\mathbf{S}$ is the set of points inside the scatterer.

Now assume that there is no scattered field before the incident field impinges upon the scatterer, such that

$$\psi_s(x, t) = 0, \quad \text{for } t < 0, \tag{4.114a}$$

$$\partial_t \psi_s(x, t) = 0, \quad \text{for } t < 0. \tag{4.114b}$$

The source s_0 of the scattered field is then replaced by $\Theta(t)s_0(x, t)$, and Eq. (4.113) becomes

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \partial_x^2\right) \psi_s(x, t) = \Theta(t)s_0(x, t). \tag{4.115}$$

Note 4.5

Analytic solutions to scattering problems are usually found by taking the incident field to be an infinite plane wave, which was thus present at $t = -\infty$ (see Appendix 4.3). In practice, the solution of Eq. (4.115) converges to that of Eq. (4.112) for “sufficiently large” t , which in practical calculations is not very large. In the next chapter this will be quantitatively clarified.

The model equation [Eq. (4.115)] is convenient for computing FDTD solutions, which require two initial fields that satisfy the boundary conditions of Eq. (4.24) on the scatterer boundary. By turning on the source of the scattered field at $t = 0$, the initial fields can be taken to be zero.

The scattered field cannot be found by using the free-space Green’s function given by Eq. (4.57) because this function does not satisfy the boundary conditions on the interface between the scatterer and the ambient medium. Usually, finding a Green’s function that satisfies boundary conditions is much more difficult than finding one in free space.

Important Points of Chapter 4

- The solution of the 1D wave equation with a source and boundary conditions is nontrivial.
- When absorption is added to the wave equation, dispersion arises.
- There are two solutions to the absorbing wave equation: complex frequency and complex wavenumber. The complex-wavenumber solution is the most physically relevant.

- We derive the scattered field wave equation.
- The wave equation derives from Newtonian mechanics, but its transformation properties lead to special relativity, which implies that the velocity of (at least some) waves must be invariant. If the speed of light is invariant in all inertial reference frames, the photon must be massless.

Appendix 4.1 The Wave Model and the Wave Equation

Waves are ubiquitous in nature, and it is remarkable that despite their great diversity the propagation of many kinds of waves is governed by the same simple equation, which we now proceed to derive.

A4.1.1 1D string

Let us begin by analyzing a displacement of a 1D uniform string under uniform tension T . Note that this assumption is only valid if the displacement of the string is small.

As shown in Fig. A4.1.1, the string is displaced from its equilibrium position by distance $\psi = \psi(x, t)$, which is a function of space x and time t .

The forces acting on a small segment of length $\Delta\ell$ are depicted the figure. Force $\mathbf{L}$ acts on the left end, and $\mathbf{R}$ acts on the right. Assuming T to be uniform throughout the string, the magnitudes of $\mathbf{L}$ and $\mathbf{R}$ are equal: $|\mathbf{L}| = |\mathbf{R}| = T$. The total force acting on $\Delta\ell$ in the ψ direction is

$$F_\psi = L_\psi + R_\psi, \quad (\text{A4.1.1})$$

where $L_\psi = T\sin\theta_L$, $R_\psi = R\sin\theta_R$, and θ_L/θ_R is the angle $\mathbf{L}/\mathbf{R}$ makes with the $+x$ axis. On the left side of $\Delta\ell$,

$$\tan\theta_L = -\left.\frac{\partial\psi}{\partial x}\right|_x, \quad (\text{A4.1.2a})$$

and on the right,

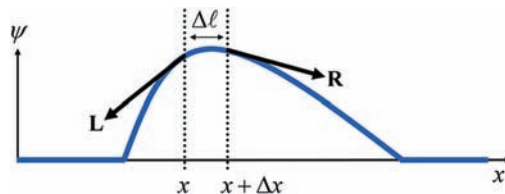


Figure A4.1.1 Forces acting on a displaced segment of string. The tension in the string is assumed to be uniform.

$$\tan \theta_R = \left. \frac{\partial \psi}{\partial x} \right|_{x+\Delta x}. \quad (\text{A4.1.2b})$$

For small displacements from equilibrium, both θ_L and θ_R are small, so $\tan \theta_L \cong \sin \theta_L$, and $\tan \theta_R \cong \sin \theta_R$. Thus,

$$\begin{aligned} F_\psi &= T(\sin \theta_L + \sin \theta_R) \\ &\cong T(\tan \theta_L + \tan \theta_R) \\ &\cong T \left(\left. \frac{\partial \psi}{\partial x} \right|_{x+\Delta x} - \left. \frac{\partial \psi}{\partial x} \right|_x \right). \end{aligned} \quad (\text{A4.1.3})$$

By definition,

$$\frac{\partial^2 \psi}{\partial x^2} = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \left(\left. \frac{\partial \psi}{\partial x} \right|_{x+\Delta x} - \left. \frac{\partial \psi}{\partial x} \right|_x \right); \quad (\text{A4.1.4})$$

therefore, in the limit $\Delta x \rightarrow 0$,

$$F_\psi = T \frac{\partial^2 \psi}{\partial x^2} \Delta x. \quad (\text{A4.1.5})$$

The acceleration of segment $\Delta \ell$ along the ψ axis is

$$a_\psi = \frac{\partial^2 \psi}{\partial t^2}. \quad (\text{A4.1.6})$$

Let the linear mass density of the string be ρ ; then its mass is $m = \rho \Delta \ell$. If both θ_L and θ_R are small, then $\Delta \ell \cong \Delta x$, and $m \cong \rho \Delta x$. From $F_\psi = m a_\psi$, we obtain

$$T \frac{\partial^2 \psi}{\partial x^2} \Delta x = (\rho \Delta x) \frac{\partial^2 \psi}{\partial t^2}, \quad (\text{A4.1.7})$$

or

$$\left[\frac{\partial^2}{\partial t^2} - \frac{T}{\rho} \frac{\partial^2}{\partial x^2} \right] \psi = 0. \quad (\text{A4.1.8})$$

By direct substitution it, can be shown that $f(x \mp t\sqrt{T/\rho})$ is a solution for arbitrary f . Defining

$$v^2 = \frac{T}{\rho}, \quad (\text{A4.1.9})$$

$f(x \pm vt)$ describes a disturbance that moves with velocity $\pm v$ along the $+x$ axis.

Wave equation

The wave equation becomes

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = 0, \quad (\text{A4.1.10})$$

where $\partial_t^2 \psi = \partial^2 \psi / \partial t^2$ and $\partial_x^2 \psi = \partial^2 \psi / \partial x^2$.

If the linear density of the string is a function of position, $\rho = \rho(x)$, then the propagation velocity, $v = v(x)$, is also a function of position.

Kinetic and potential energy density

The kinetic energy density of the string is obviously

$$K(x, t) = \frac{1}{2} \rho(x) [\partial_t \psi(x, t)]^2. \quad (\text{A4.1.11})$$

The potential energy is much more difficult to determine. Here we give a simple derivation that is adequate for our purposes. Let us assume the string to be elastic and the tension constant. The length of the string segment between x and $x + \Delta x$ is $s(\partial_x \psi) = \sqrt{\Delta x^2 + (\Delta x \partial_x \psi)^2}$. The work needed to stretch the segment from length $s(0) = \Delta x$ to length $s(\partial_x \psi)$ is $\Delta V = T \Delta s$, where $\Delta s = \sqrt{\Delta x^2 + (\Delta x \partial_x \psi)^2} - \Delta x$ is assumed to be small. Expanding Δs in a Taylor series, we obtain the potential energy density:

$$V(x, t) = \frac{1}{2} T (\partial_x \psi)^2. \quad (\text{A4.1.12})$$

The above is a simplified derivation that avoids certain devilish details. More complete and rigorous discussions can be found in Refs. 1 and 2.

Note A4.1.1

While the potential energy of a simple harmonic oscillator is a function of its displacement from equilibrium, that of a wave on a string is a function of the string's deformation.

The energy density is $E = K + V$, which for a harmonic wave $\psi(x, t) = A \sin(kx - \omega t)$ is

$$E(x, t) = \rho \omega^2 A^2 \cos^2(kx - \omega t), \quad (\text{A4.1.13})$$

where $\omega = kv$. Notice that the energy density oscillates with angular frequency 2ω . It is not constant because the wave transports energy.

A4.1.2 Two and three dimensions

In two and three dimensions, the wave equation is

$$(\partial_t^2 - v^2 \nabla^2) \psi(\mathbf{x}, t) = 0, \quad (\text{A4.1.14})$$

where $\nabla^2 = \partial_x^2 + \partial_y^2$, and $\mathbf{x} = (x, y)$ in two dimensions; and $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$, and $\mathbf{x} = (x, y, z)$ in three.

A4.1.3 Wave equation with a source

Ultimately, waves are generated by sources. The wave equation with a source is

$$(\partial_t^2 - v^2 \nabla^2) \psi(\mathbf{x}, t) = s(\mathbf{x}, t), \quad (\text{A4.1.15})$$

where the source s is a function of position and time. Equation (A4.1.14) is called the *homogeneous* wave equation, while Eq. (A4.1.15) is the *inhomogeneous* wave equation.

A4.1.4 Damped wave equation with a source

When an object slides on a rough surface with velocity u , a good approximation to the sliding frictional force opposing its motion is $f = -\alpha u$, where α is the coefficient of friction. Similarly, a good model for many damped waves is

$$\partial_t^2 \psi(\mathbf{x}, t) = v^2 \nabla^2 \psi(\mathbf{x}, t) - 2\alpha \partial_t \psi(\mathbf{x}, t), \quad (\text{A4.1.16})$$

or

$$(\partial_t^2 + 2\alpha \partial_t - v^2 \nabla^2) \psi(\mathbf{x}, t) = 0. \quad (\text{A4.1.17})$$

For mathematical convenience, it is conventional to insert a factor of 2 in Eq. (A4.1.16). Adding a source term, we obtain

$$(\partial_t^2 + 2\alpha \partial_t - v^2 \nabla^2) \psi(\mathbf{x}, t) = s(\mathbf{x}, t). \quad (\text{A4.1.18})$$

Appendix 4.2 Transformation of the Wave Equation and Special Relativity

It is remarkable that the wave equation, which derives from classical Newtonian mechanics, leads to special relativity. Although classical mechanics is an excellent approximation for many purposes, it is not self-consistent. The wave equation is not invariant under a Galilean transformation. By requiring it to be invariant under transformation from one inertial reference frame to another, we derive the Lorentz transformation and deduce some of the most important results of special relativity. Finally, we show that although the photon is massless, it carries both energy and momentum.

A4.2.1 Galilean transformation

Let $S(x, y, t)$ be a space–time coordinate system that we call “stationary,” and let $S'(x', y', t')$ be a coordinate system that moves with velocity v along the x axis of S , as shown in Fig. A4.2.1.

Let the origins of both systems coincide at $t = t' = 0$. In Newtonian (or classical mechanics), the relationship between S and S' is given by the Galilean transformation

$$x' = x - vt, \quad (\text{A4.2.1a})$$

$$t' = t. \quad (\text{A4.2.1b})$$

Perpendicular to the relative motion, $y' = y$ and $z' = z$. It is convenient to express the Galilean transformation in matrix form as

$$\begin{bmatrix} x' \\ t' \end{bmatrix} = G(v) \begin{bmatrix} x \\ t \end{bmatrix}, \quad (\text{A4.2.2})$$

where

$$G(v) = \begin{bmatrix} 1 & -v \\ 0 & 1 \end{bmatrix}. \quad (\text{A4.2.3})$$

The transformations $y' = y$ and $z' = z$ are omitted. It is easy to verify that the conservation of momentum and energy holds under Galilean transformation.

Note A4.2.1

Galilean transformations form a Lie group, and $G(v_2)G(v_1) = G(v_1 + v_2)$.

A4.2.2 General transformation of the wave equation

Before examining its properties under a Galilean transformation, let us first see how the wave equation

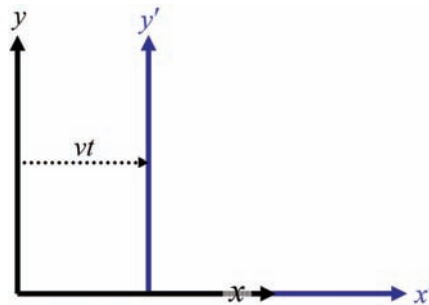


Figure A4.2.1 Reference frame $S'(x', y')$ moves with velocity v relative to $S(x, y)$.

$$(\partial_t^2 - c^2 \partial_x^2) \psi(x, t) = 0 \quad (\text{A4.2.4})$$

changes under a general 1D coordinate transformation of the form

$$x' = x'(x, t), \quad (\text{A4.2.5a})$$

$$t' = t'(x, t). \quad (\text{A4.2.5b})$$

(Here, c is not necessarily the speed of light.) Expressing $\partial\psi(x, t)/\partial x$ in terms of $\partial\psi'(x', t')/\partial x'$ and $\partial\psi'(x', t')/\partial t'$, we obtain

$$\frac{\partial}{\partial x} \psi(x, t) = \frac{\partial x'}{\partial x} \frac{\partial}{\partial x'} \psi'(x', t') + \frac{\partial t'}{\partial x} \frac{\partial}{\partial t'} \psi'(x', t'), \quad (\text{A4.2.6a})$$

or

$$\partial_x \psi(x, t) = (\partial_t x' \partial_{x'} + \partial_t t' \partial_{t'}) \psi'(x', t'). \quad (\text{A4.2.6b})$$

Similarly,

$$\partial_t \psi(x, t) = (\partial_t x' \partial_{x'} + \partial_t t' \partial_{t'}) \psi'(x', t'). \quad (\text{A4.2.7})$$

Thus,

$$\begin{aligned} \partial_x^2 \psi(x, t) &= (\partial_x x' \partial_{x'} + \partial_x t' \partial_{t'})^2 \psi'(x', t') \\ &= ([\partial_x x']^2 \partial_{x'}^2 + [\partial_x t']^2 \partial_{t'}^2 + 2[\partial_x x'][\partial_x t'] \partial_{x'} \partial_{t'}) \psi'(x', t'), \end{aligned} \quad (\text{A4.2.8})$$

$$\partial_t^2 \psi(x, t) = ([\partial_t x']^2 \partial_{x'}^2 + [\partial_t t']^2 \partial_{t'}^2 + 2[\partial_t x'][\partial_t t'] \partial_{x'} \partial_{t'}) \psi'(x', t'). \quad (\text{A4.2.9})$$

A4.2.3 Galilean transformation of the wave equation

Inserting the Galilean transformation [Eq. (A4.2.1)] into Eqs. (A4.2.8) and (A4.2.9), we find that

$$\partial_x^2 \psi(x, t) = \partial_{x'}^2 \psi(x', t'), \quad (\text{A4.2.10})$$

and

$$\partial_t^2 \psi(x, t) = (\partial_{t'}^2 + v^2 \partial_{x'}^2 - 2v \partial_t \partial_{x'}) \psi'(x', t'). \quad (\text{A4.2.11})$$

A wave in S propagates according to the wave equation [Eq. (A4.2.4)], but in S' it obeys

$$[\partial_{t'}^2 - (c^2 - v^2)\partial_{x'}^2 - 2v\partial_{t'}\partial_{x'}]\psi'(x', t') = 0. \quad (\text{A4.2.12})$$

Thus, the wave equation is not invariant under Galilean transformation because its form is different in S' .

Classical Doppler shift

The transformed wave [Eq. (A4.2.12)] can be factored into

$$[\partial_{t'} + (c - v)\partial_{x'}][\partial_{t'} + (c + v)\partial_{x'}]\psi'(x', t') = 0, \quad (\text{A4.2.13})$$

which implies the two one-way wave equations:

$$[\partial_{t'} + (c - v)\partial_{x'}]\psi'(x', t') = 0, \quad (\text{A4.2.14a})$$

$$[\partial_{t'} + (c + v)\partial_{x'}]\psi'(x', t') = 0. \quad (\text{A4.2.14b})$$

The solution of Eq. (A4.2.14a) is $\psi'(x', t') = f[x' - (c - v)t']$, which is a wave form that propagates in the $+x'$ direction with velocity $c - v$, where f is an arbitrary function. Similarly, the solution of Eq. (A4.2.14b) is $\psi'(x', t') = f[x' + (c + v)t']$, which is a wave propagating with velocity $c + v$ along $-x'$. Thus, in S' , waves propagate with different velocities in different directions. Wave velocity is the product of wavelength λ and frequency ν ; since λ is the same in both S and S' , the frequencies of the forward- and backward-moving waves are $\nu_{\pm} = (c \mp v)/\lambda$, which is the classical Doppler shift.

A4.2.4 Lorentz transformation

Numerous experiments have shown that the speed of light is constant regardless of the relative motion of the source and observer so the classical Doppler shift is wrong for light. Thus, it is disturbing that the wave equation for light should be different in different reference frames. Additionally, it raises the embarrassing question: Is the wave equation [Eq. (A4.2.4)] valid only in some chosen reference frame? In addition, Maxwell's equations, which reduce to the wave equation in free space, would also have to depend on the reference frame.

If we believe the laws of physics to be the same in any inertial reference frame, then there are two choices: (1) The wave equation is correct, and the Galilean transformation is wrong, or (2) the wave equation does not apply to electromagnetic waves, and the Galilean transformation is correct. Experimental evidence together with a belief that the universe must be “simple” lead us to the first choice.

We now proceed to find a transformation under which the wave equation is invariant. The simplest, most general, linear coordinate transformation is

$$\begin{bmatrix} x' \\ t' \end{bmatrix} = L(v) \begin{bmatrix} x \\ t \end{bmatrix}, \quad (\text{A4.2.15})$$

where

$$L(v) = \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix}. \quad (\text{A4.2.16})$$

We now seek L such that the form of the wave equation is the same in both S and S' ; that is,

$$(\partial_{t'}^2 - c^2 \partial_{x'}^2) \psi'(x', t') = 0. \quad (\text{A4.2.17})$$

Since the Galilean transformation seems to be correct at low relative velocities, the new transformation [Eq. (A4.2.15)] ought to reduce to the Galilean transformation. Thus,

$$\lim_{v \rightarrow 0} \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix} = \begin{bmatrix} 1 & -v \\ 0 & 1 \end{bmatrix}. \quad (\text{A4.2.18})$$

We thus postulate the new transformation to be of the form

$$\begin{bmatrix} x' \\ t' \end{bmatrix} = \begin{bmatrix} \gamma(x - vt) \\ \gamma(\alpha x + t) \end{bmatrix} = \begin{bmatrix} \gamma & -\gamma v \\ \gamma \alpha & \gamma \end{bmatrix} \begin{bmatrix} x \\ t \end{bmatrix}, \quad (\text{A4.2.19})$$

where γ and α are unknown parameters to be found. The limit given in Eq. (A4.2.18) implies that

$$\lim_{v \rightarrow 0} \gamma = 1, \quad (\text{A4.2.20a})$$

$$\lim_{v \rightarrow 0} \alpha = 0. \quad (\text{A4.2.20b})$$

Using the transformation [Eq. (A4.2.19)], we take $x'(x, t) = \gamma(x - vt)$ in Eq. (A4.2.8) and $t'(x, t) = \gamma(\alpha x + t)$ in Eq. (A4.2.9) to obtain

$$\partial_x^2 \psi(x, t) = \left[\alpha^2 \gamma^2 \partial_t^2 + \gamma^2 \partial_{x'}^2 + 2\alpha \gamma^2 \partial_{t'} \partial_{x'} \right] \psi'(x', t'), \quad (\text{A4.2.21a})$$

$$\partial_t^2 \psi(x, t) = \left[\gamma^2 \partial_{t'}^2 + \gamma^2 v^2 \partial_{x'}^2 - 2\gamma^2 v \partial_{t'} \partial_{x'} \right] \psi'(x', t'). \quad (\text{A4.2.21b})$$

Thus, in S' , the wave equation becomes

$$\left[\gamma^2(1 - \alpha^2 c^2) \partial_{t'}^2 - \gamma^2(c^2 - v^2) \partial_{x'}^2 - 2\gamma^2(\alpha c^2 + v) \partial_{t'} \partial_{x'} \right] \psi'(x', t') = 0. \quad (\text{A4.2.22})$$

Requiring Eq. (A4.2.22) to be equivalent to Eq. (A4.2.17),

$$\left[\gamma^2(1 - \alpha^2 c^2) \partial_{t'}^2 - \gamma^2(c^2 - v^2) \partial_{x'}^2 - 2\gamma^2(\alpha c^2 + v) \partial_{t'} \partial_{x'} \right] = [\partial_{t'}^2 - c^2 \partial_{x'}^2], \quad (\text{A4.2.23})$$

and comparing the $\partial_{x'}^2$ terms and $\partial_{t'}^2$ terms, we find that

$$\gamma^2(c^2 - v^2) = c^2 \Rightarrow \gamma = \frac{1}{\sqrt{1 - v^2/c^2}}, \quad (\text{A4.2.24})$$

$$(1 - \alpha^2 c^2) = \frac{1}{\gamma^2} \Rightarrow \alpha = -\frac{v}{c^2}. \quad (\text{A4.2.25})$$

It is easy to verify that γ and α satisfy the limits given in Eq. (A4.2.20). The wave equation is thus invariant under what is called the Lorentz transformation:

$$\begin{bmatrix} x' \\ t' \end{bmatrix} = \gamma \begin{bmatrix} 1 & -v \\ -v/c^2 & 1 \end{bmatrix} \begin{bmatrix} x \\ t \end{bmatrix}. \quad (\text{A4.2.26})$$

In the limit $v \rightarrow 0$, the Lorentz transformation reduces to the Galilean transformation.

Note A4.2.2

Lorentz transformations also form a Lie group.

An important consequence of the Lorentz transformation is that nothing can travel faster than the velocity of light. It is easy to see that $\lim_{v \rightarrow 0} \gamma = \infty$, and $v > c$ implies that γ is imaginary. Since x' and t' must be real and finite, we reject both infinite and imaginary values of γ and hence arrive at the constraint $v < c$.

We rejected the Galilean transformation [choice (2) above] because it implied a special chosen reference frame in which the wave equation holds. However, now the speed of light appears to be the chosen velocity, which sets a universal speed limit. We accept this situation because the vacuum speed of light is, so far, the fastest velocity known, and numerous experiments have shown the validity of relativity theory.

A4.2.5 Transformation of velocity

If S' moves with velocity v relative to S , then S moves with velocity $-v$ relative to S' , so the Lorentz transformation from S' to S is

$$\begin{bmatrix} x \\ t \end{bmatrix} = \gamma \begin{bmatrix} 1 & v \\ v/c^2 & 1 \end{bmatrix} \begin{bmatrix} x' \\ t' \end{bmatrix}. \quad (\text{A4.2.27})$$

If an object moves with velocity $u' = \Delta x'/\Delta t'$ relative to S' , from Eq. (A4.2.27), its velocity relative to S is

$$\begin{aligned} u &= \frac{\Delta x}{\Delta t} = \frac{\Delta x' + v\Delta t'}{\Delta t' + v\Delta x'/c^2} \\ &= \frac{v + u'}{1 + u'v/c^2}. \end{aligned} \quad (\text{A4.2.28})$$

Taking $u' = c$ gives $u' = c$, so the velocity of light is the same in both S and S' . On the other hand, in the limit $u'v/c^2 \rightarrow 0$, $u \rightarrow u' + v$, which agrees with the Galilean transformation.

A4.2.6 Transformation of acceleration

Let an object be instantaneously at rest in S' , and let its velocity be $u' = 0$ and its acceleration be $a' = \Delta u'/\Delta t'$. Thus, it moves with velocity v in S . Its acceleration in S is $a = \Delta u/\Delta t$, where $\Delta u = (du/du')\Delta u'$, and $\Delta t = \gamma\Delta t'$ [not $\Delta t = \gamma(v\Delta x'/c^2 + \gamma\Delta t')$ because $\Delta x' = u'\Delta t'$ and $u' = 0$]. Therefore,

$$a = \frac{a'}{\gamma^3}. \quad (\text{A4.2.29})$$

A4.2.7 Relativistic momentum

In one dimension, when a constant force F acts on a mass m , it produces acceleration $a = du/dt$ given by

$$F = m \frac{du}{dt}, \quad (\text{A4.2.30})$$

where u is its velocity. Integrating with respect to time, we find that u eventually exceeds the speed of light and becomes infinite, which (we believe) is physically impossible. Thus, Eq. (A4.2.30) cannot be correct. Using Newton's definition of momentum

$$p = mu, \quad (\text{A4.2.31})$$

Eq. (A4.2.30) can be expressed in the alternative form

$$F = \frac{d}{dt}p. \quad (\text{A4.2.32})$$

Assuming Eq. (A4.2.32) to be correct in all inertial reference frames, let us modify the definition of momentum in such a way that it reduces to the classical definition at low velocities. We require that

$$\lim_{u \rightarrow 0} p = mu. \quad (\text{A4.2.33})$$

Let a force act upon mass m , which is instantaneously at rest in S' so that its velocity is $u' = 0$, and its acceleration is a' . Since Eq. (A4.2.30) is assumed to be valid in the limit $u' \rightarrow 0$, the force acting in S' is $F' = ma'$. On the other hand, in S , m moves with velocity $u = v$, so the force F in S is given by Eq. (A4.2.32). Relative to S , the acceleration a of m is

$$a = \frac{dv}{dt} = \frac{a'}{\gamma^3} \quad (\text{A4.2.34})$$

from Eq. (A4.2.29). Hence,

$$\gamma^3 \frac{dv}{dt} = \frac{d}{dt}(\gamma v) = a'. \quad (\text{A4.2.35})$$

It is easy to show that $\gamma^3 dv/dt = d(\gamma v)/dt$. Thus,

$$\begin{aligned} F' &= ma' \\ &= m \frac{d}{dt}(\gamma v). \end{aligned} \quad (\text{A4.2.36})$$

Assuming that force F in S is the same as force F' in S' ,

$$F = F', \quad (\text{A4.2.37})$$

then

$$\begin{aligned} F &= \frac{d}{dt}p \\ &= m \frac{d}{dt}(\gamma v), \end{aligned} \quad (\text{A4.2.38})$$

where $v = v(t)$ and $\gamma = \gamma[v(t)]$. Thus,

$$\frac{d}{dt}p = m \frac{d}{dt}(\gamma v). \quad (\text{A4.2.39})$$

Taking $p(0) = 0$ and $v(0) = 0$, and integrating with respect to t , we find that

$$p = \gamma m v. \quad (\text{A4.2.40})$$

The relativistic momentum given by Eq. (A4.2.38) thus reduces to the classical expression $p = mv$ for $v \ll c$ because $\gamma \rightarrow 1$.

A4.2.8 Relativistic energy

In Newtonian mechanics, the kinetic energy K of a mass m moving with velocity u is

$$K = \frac{1}{2} m u^2. \quad (\text{A4.2.41})$$

Let us now seek the correct relativistic expression for kinetic energy. If force F causes mass m to move distance dx , it increases its kinetic energy by $dK = Fdx$. If m moves with velocity v , then

$$F v = \frac{d}{dt} K. \quad (\text{A4.2.42})$$

From Eq. (A4.2.38),

$$m v \frac{d}{dt} (\gamma v) = \frac{d}{dt} K. \quad (\text{A4.2.43})$$

It is easy to show that

$$c \frac{d}{dt} (\gamma v) = c^3 \frac{d}{dt} \gamma; \quad (\text{A4.2.44})$$

therefore,

$$\frac{d}{dt} K = m c^2 \frac{d}{dt} \gamma. \quad (\text{A4.2.45})$$

Integrating both sides with respect to t , we find that

$$K(t) - K(0) = m c^2 [\gamma(t) - \gamma(0)]. \quad (\text{A4.2.46})$$

At $t = 0$, taking $v = 0$ and $K(0) = 0$, and using the fact that $\gamma(v = 0) = 1$, the relativistic kinetic energy is

$$K = (\gamma - 1) m c^2. \quad (\text{A4.2.47})$$

In the limit $v \ll c$, it is easy to show that $K \rightarrow (1/2) m v^2$.

In general, the total energy E is the sum of the potential energy and the kinetic energy. In the absence of a potential, the change in total energy equals the change in kinetic energy; thus, Eq. (A4.2.46) becomes

$$\begin{aligned}
 E|_v - E|_{v=0} &= E|_v - E|_{v=0} \\
 &= \gamma(v)mc^2 - \gamma(0)mc^2.
 \end{aligned}
 \tag{A4.2.48}$$

Since $\gamma(0) = 1$, Einstein concluded that $E|_{v=0} = mc^2$ so that an object at rest has an intrinsic energy—called its rest energy—due to its mass. Adding the rest energy to the kinetic energy [Eq. (A4.2.47)] (and assuming no potential energy), an object moving with velocity v has total energy

$$E = \gamma(v)mc^2. \tag{A4.2.49}$$

A4.2.9 Invariants under the Lorentz transformation

Let $\mathbf{V} = (V_x, V_y)$ be some vector. When the coordinate system is rotated or translated, its components change as $(V_x, V_y) \rightarrow (V'_x, V'_y)$, but the magnitude of $\mathbf{V}$, $|\mathbf{V}| = \sqrt{V_x^2 + V_y^2}$, remains the same; thus, $V_x^2 + V_y^2 = V'^2_x + V'^2_y$. $|\mathbf{V}|$ is said to be an *invariant* with respect to rotation and translation.

What are the invariants of the Lorentz transformation? Let us define $\mathbf{P} = (ct, x)$ to be a space–time position vector in reference frame S , as shown in Fig. A4.2.2. Space–time vectors are sometimes called “events.” Taking $\mathbf{P}_1 = (ct_1, x_1)$ and $\mathbf{P}_2 = (ct_2, x_2)$, let vector $\Delta\mathbf{s} = \mathbf{P}_2 - \mathbf{P}_1$, and define its magnitude by $|\Delta\mathbf{s}|^2 = (ct_2 - ct_1)^2 - (x_2 - x_1)^2$.

Note A4.2.3

A space with this definition of magnitude is called a Minkowski space. In four dimensions (three of space and one of time), $\mathbf{P}_1$, $\mathbf{P}_2$, and $\Delta\mathbf{s}$ are called four-vectors.

If (x, t) and (x', t') are related by a Lorentz transformation, it is easy to show that

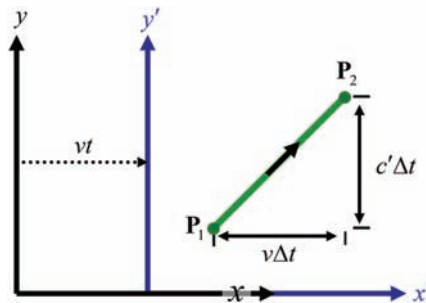


Figure A4.2.2 Light propagates along the y' axis with velocity c' ; in S it moves at an angle relative to the y axis.

$$(ct_2 - ct_1) - (x_2 - x_1)^2 = (ct'_2 - ct'_1)^2 - (x'_2 - x'_1)^2. \quad (\text{A4.2.50})$$

Hence, $|\Delta \mathbf{s}| = |\Delta \mathbf{s}'|$ is invariant under a Lorentz transformation, and $|\Delta \mathbf{s}|$ is called a *Lorentz invariant*.

Similarly, we define the energy momentum vector $\mathbf{p} = (E/c, p)$, called the *four-momentum* (in three spatial dimensions), and its magnitude by $|\mathbf{p}|^2 = (E/c)^2 - p^2$. Using Eqs. (A4.2.40) and (A4.2.49), we find that

$$p' = \gamma(p - vt), \quad (\text{A4.2.51a})$$

$$E'/c = \gamma \left(E/c - \frac{vp}{c^2} \right). \quad (\text{A4.2.51b})$$

Thus, with the correspondences $E/c \leftrightarrow t$ and $p \leftrightarrow x$, the components of the energy-momentum vector in S and S' are related by the Lorentz transformation given by Eq. (A4.2.27). It is then easy to show that

$$|\mathbf{p}|^2 = |\mathbf{p}'|^2 = m^2 c^2. \quad (\text{A4.2.52})$$

Thus, the magnitude of four-momentum and (by implication) mass is a Lorentz invariant.

Finally, let us re-examine Eq. (A4.2.49). It might seem that $m = 0$, which implies that $E = 0$, but this is not true. Rewriting Eq. (A4.2.51) gives

$$E^2 - p^2 c^2 = m^2 c^4. \quad (\text{A4.2.53})$$

Therefore, $m = 0$, which implies that

$$E = pc. \quad (\text{A4.2.54})$$

This result tells us that a massless particle, such as the photon, can carry both momentum and energy. It has been experimentally confirmed that light does indeed carry both momentum and energy.

Appendix 4.3 Reflection and Transmission of Layered Structures

The propagation of waves in layered structures is of great technological importance, and many specialist books and papers are extant. The purpose of this section is simply to derive a few analytic solutions against which numerical algorithms can later be checked.

We seek solutions of

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \partial_x^2 \right) \psi(x, t) = 0, \quad (\text{A4.3.1})$$

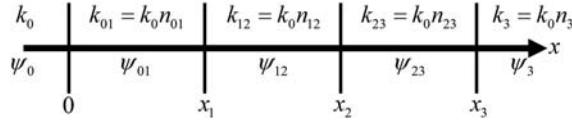


Figure A4.3.1 Solutions and their wavenumbers in each section of a multilayer structure.

where n can be complex if one of the layers is an absorbing material (see Section 4.3.2).

Consider the 1D layered structure depicted in Fig. A4.3.1 and defined by

$$\begin{aligned} n &= 1 & \text{for } x &\leq 0, \\ n &= n_{01} & \text{for } 0 < x &\leq x_1, \\ n &= n_{12} & \text{for } x_1 < x &\leq x_2, \\ n &= n_{23} & \text{for } x_2 < x &\leq x_3, \\ n &= n_3 & \text{for } x &> x_3, \end{aligned} \quad (\text{A4.3.2})$$

where $n_{01}, n_{12}, \dots$, are the refractive indices relative to the refractive index of the material in the $x \leq 0$ region. We can always set $n = 1$, even if the physical refractive index of the $x \leq 0$ material $\neq 1$.

Taking the time dependence of the wave field to be $e^{-i\omega t}$ (it could equally well be $e^{+i\omega t}$), let an incident wave $\psi_i = e^{i(k_0 x - \omega t)}$ impinge on the structure from the $-x$ direction, where $k_0 = \omega/\nu_0$. In the $x \leq 0$ region, the field $\psi_0 = \varphi_0 e^{-i\omega t}$ is the superposition of the incident field and a reflected field of amplitude r ; thus,

$$\varphi_0 = e^{ik_0 x} + r e^{-ik_0 x} \quad \text{for } x \leq 0. \quad (\text{A4.3.3a})$$

In an interior layer of refractive index n , waves can reflect from both interfaces, so the field is a superposition of two waves propagating in the $\pm x$ directions of the form $\psi(x, t) = \varphi(x) e^{-i\omega t}$, where $\varphi(x) = a_+ e^{ikx} + a_- e^{-ikx}$, and $k = nk_0$. Thus,

$$\varphi_{01} = a_{01}^+ e^{ik_{01} x} + a_{01}^- e^{-ik_{01} x}, \quad \text{for } 0 < x \leq x_1. \quad (\text{A4.3.3b})$$

$$\varphi_{12} = a_{12}^+ e^{ik_{12} x} + a_{12}^- e^{-ik_{12} x}, \quad \text{for } x_1 < x \leq x_2, \quad (\text{A4.3.3c})$$

$$\varphi_{23} = a_{23}^+ e^{ik_{23} x} + a_{23}^- e^{-ik_{23} x}, \quad \text{for } x_2 < x \leq x_3, \quad (\text{A4.3.3d})$$

where the wavenumber in layer i ($i = 01, 12, 23, 3$) is $k_i = n_i k_0$. The wave that is finally transmitted through the structure moves in the $+x$ direction and is thus

$$\varphi_3 = \tau e^{ik_3 x}, \quad \text{for } x > x_3, \quad (\text{A4.3.3e})$$

where τ is its amplitude.

We now proceed to find r and τ by using the conditions that both ψ and $\partial_x \psi$ (and by implication, φ and $\partial_x \varphi$) must be continuous at the interfaces. At $x = 0$ we have

$$1 + r = a_{01}^+ + a_{01}^-, \quad (\text{A4.3.4a})$$

$$k_0(1 - r) = k_{01}(a_{01}^+ - a_{01}^-). \quad (\text{A4.3.4b})$$

Defining

$$\mathbf{A}(k, x) = \begin{bmatrix} e^{ikx} & e^{-ikx} \\ ke^{ikx} & -ke^{-ikx} \end{bmatrix}, \quad (\text{A4.3.5})$$

Eq. (A4.3.4) can be expressed in matrix form as

$$\mathbf{A}(k_0, 0)\Psi_0 = \mathbf{A}(k_{01}, 0)\Psi_{01}, \quad (\text{A4.3.6})$$

where

$$\Psi_0 = \begin{bmatrix} 1 \\ r \end{bmatrix}, \Psi_{01} = \begin{bmatrix} a_{01}^+ \\ a_{01}^- \end{bmatrix}. \quad (\text{A4.3.7})$$

Similarly, at the x_{1-} , x_{2-} , and x_{3-} boundaries, we have

$$\mathbf{A}(k_{01}, x_1)\Psi_{01} = \mathbf{A}(k_{12}, x_1)\Psi_{12}, \quad (\text{A4.3.8})$$

$$\mathbf{A}(k_{12}, x_2)\Psi_{12} = \mathbf{A}(k_{23}, x_2)\Psi_{23}, \quad (\text{A4.3.9})$$

$$\mathbf{A}(k_{23}, x_3)\Psi_{23} = \mathbf{A}(k_3, x_3)\Psi_3, \quad (\text{A4.3.10})$$

where

$$\Psi_{12} = \begin{bmatrix} a_{12}^+ \\ a_{12}^- \end{bmatrix}, \Psi_{23} = \begin{bmatrix} a_{23}^+ \\ a_{23}^- \end{bmatrix}, \Psi_3 = \begin{bmatrix} \tau \\ 0 \end{bmatrix}. \quad (\text{A4.3.11})$$

Solving Eq. (A4.3.6) for Ψ_0 , Eq. (A4.3.8) for Ψ_{01} , Eq. (A4.3.9) for Ψ_{12} , etc., we obtain

$$\Psi_0 = \mathbf{A}^{-1}(k_0, 0)\mathbf{A}(k_{01}, 0)\Psi_{01}, \quad (\text{A4.3.12a})$$

$$\Psi_{01} = \mathbf{A}^{-1}(k_{01}, x_1)\mathbf{A}(k_{12}, x_1)\Psi_{12}, \quad (\text{A4.3.12b})$$

$$\Psi_{12} = \mathbf{A}^{-1}(k_{12}, x_2)\mathbf{A}(k_{23}, x_2)\Psi_{23}, \quad (\text{A4.3.12c})$$

$$\Psi_{23} = \mathbf{A}^{-1}(k_{23}, x_3)\mathbf{A}(k_3, x_3)\Psi_3. \quad (\text{A4.3.12d})$$

Thus,

$$\begin{aligned}\Psi_0 &= \mathbf{A}^{-1}(k_0, 0) \mathbf{A}(k_{01}, 0) \mathbf{A}^{-1}(k_{01}, x_1) \mathbf{A}(k_{12}, x_1) \mathbf{A}^{-1}(k_{12}, x_2) \mathbf{A}(k_{23}, x_2) \\ &\quad \bullet \mathbf{A}^{-1}(k_{23}, x_3) \mathbf{A}(k_3, x_3) \Psi_3.\end{aligned}\quad (\text{A4.3.13})$$

The inverse of $\mathbf{A}(k, x)$ is

$$\mathbf{A}^{-1}(k, x) = \frac{1}{2k} \begin{bmatrix} k e^{-ikx} & e^{-ikx} \\ k e^{ikx} & -e^{ikx} \end{bmatrix}. \quad (\text{A4.3.14})$$

Defining

$$\begin{aligned}\mathbf{B} &= \mathbf{A}^{-1}(k_0, 0) \mathbf{A}(k_{01}, 0) \mathbf{A}^{-1}(k_{01}, x_1) \mathbf{A}(k_{12}, x_1) \mathbf{A}^{-1}(k_{12}, x_2) \mathbf{A}(k_{23}, x_2) \\ &\quad \bullet \mathbf{A}^{-1}(k_{23}, x_3) \mathbf{A}(k_3, x_3),\end{aligned}\quad (\text{A4.3.15})$$

we obtain

$$\begin{bmatrix} 1 \\ r \end{bmatrix} = \mathbf{B} \begin{bmatrix} \tau \\ 0 \end{bmatrix}. \quad (\text{A4.3.16})$$

Solving Eq. (A4.3.16) for r and τ , we find that

$$\tau = \frac{1}{B_{11}}, r = \frac{B_{21}}{B_{11}}. \quad (\text{A4.3.17})$$

This procedure can be straightforwardly generalized to any number of layers, but when there are too many layers, computational troubles can arise due to round-off and truncation errors.

A4.3.1 Single layer

A case of particular interest is a single layer with the same medium outside the layer. Let $n = 1$ for $x \leq 0$, $n = n_s$ for $0 < x < a$, and $n = 1$ for $x > a$ (see Figs. A4.3.2 and A4.3.3). Then, $k_{01} = n_s k_0$, and $\mathbf{B} = \mathbf{A}^{-1}(k_0, 0) \mathbf{A}(n_s k_0, 0) \mathbf{A}^{-1}(n_s k_0, a) \mathbf{A}(k_0, a)$. Evaluating B_{11} and B_{21} , we find that

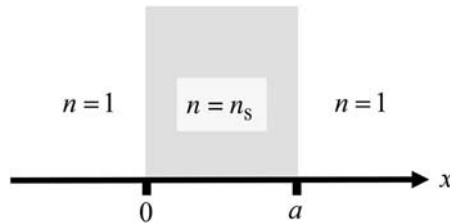


Figure A4.3.2 Layer of width a and refractive index n_s relative to the ambient medium.

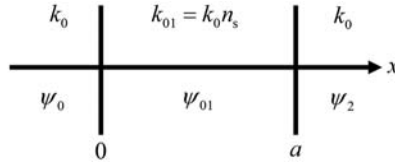


Figure A4.3.3 Wavenumbers of the solutions in a single layer of refractive index n_s .

$$\tau = \frac{2n_s e^{-ik_0 a}}{2n_s \cos(n_s k_0 a) - i(n_s^2 + 1) \sin(n_s k_0 a)}, \quad (\text{A4.3.18})$$

$$r = \frac{i(n_s^2 - 1) \sin(n_s k_0 a)}{2n_s \cos(n_s k_0 a) - i(n_s^2 + 1) \sin(n_s k_0 a)}. \quad (\text{A4.3.19})$$

It is also interesting to solve for the interior field ψ_{01} . Solving Eq. (A4.3.6) for Ψ_{01} using $k_{01} = n_s k_0$, we find that

$$\Psi_{01} = \mathbf{A}^{-1}(n_s k_0, 0) \mathbf{A}(k_0, 0) \Psi_0. \quad (\text{A4.3.20})$$

Using Eqs. (A4.3.5) and (A4.3.14), we find that

$$a_{01}^{\pm} = \left(\frac{n_s \pm 1}{2n_s} \right) + \left(\frac{n_s \pm 1}{2n_s} \right) r. \quad (\text{A4.3.21})$$

Appendix 4.4 Green's Function for the 1D Wave Equation

Using a Green's function, we can construct analytic solutions to the wave equation with a source:

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = s(x, t). \quad (\text{A4.4.1})$$

By definition, a Green's function G is the solution of

$$(\partial_t^2 - v^2 \partial_x^2) G(x, t; x', t') = \delta(x - x') \delta(t - t'). \quad (\text{A4.4.2})$$

Physically, it is the field at (x, t) due to a space–time point source at (x', t') . Using the properties of δ functions, it can be verified by direct substitution that the solution of Eq. (A4.4.1) is

$$\psi(x, t) = \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dx' G(x, x', t, t') s(x', t'). \quad (\text{A4.4.3})$$

Because it must satisfy the same boundary and initial conditions of the differential equation itself, the Green's function is often difficult—if not impossible—to find analytically, except in a few special cases. These special cases can, however, give us deep insight into the physics, and analytic

solutions of solvable problems can be compared with numerical solutions to evaluate the accuracy of algorithms.

We now proceed to derive the Green's function with respect to the wave equation for several cases of interest.

A4.4.1 Green's function in unbounded space

Since waves from a point source propagate isotropically outward, we assume G to be a function of the space–time separation $(\chi, \tau) = (x - x', t - t')$ of source point (x', t') and the observation point (x, t) so that

$$\begin{aligned} G &= G(x, t; x', t') \\ &= G(x - x', t - t'). \end{aligned} \quad (\text{A4.4.4})$$

Equation (A4.4.2) thus becomes

$$(\partial_\tau^2 - v^2 \partial_\chi^2) G(\chi, \tau) = \delta(\chi) \delta(\tau), \quad (\text{A4.4.5})$$

which is equivalent to

$$(\partial_t^2 - v^2 \partial_x^2) G(x - x', t - t') = \delta(x - x') \delta(t - t') \quad (\text{A4.4.6})$$

because $\partial_x = \partial_\chi$, and $\partial_t = \partial_\tau$ because (x', t') is fixed.

We first solve Eq. (A4.4.5) at $\chi \neq 0$ and $\tau \neq 0$, where the equation becomes

$$(\partial_\tau^2 - v^2 \partial_\chi^2) G(\chi, \tau) = 0. \quad (\text{A4.4.7})$$

A general solution of Eq. (A4.4.7) is

$$G(\chi, \tau) = f(v\tau - \chi) + g(v\tau + \chi), \quad (\text{A4.4.8})$$

where $v > 0$, and f and g are arbitrary functions. In isotropic space, the wave function is symmetric about a point source at $\chi = 0$, so we take $f = g$. Physically, a wave always propagates away from its source, so for $\chi > 0$, $G(\chi, \tau) = f(v\tau - \chi)$, and for $\chi < 0$, $G(\chi, \tau) = f(v\tau + \chi)$. The solution for all $\chi \neq 0$ can be compactly expressed as

$$G(\chi, \tau) = f(v\tau - |\chi|). \quad (\text{A4.4.9})$$

The problem now reduces to finding f . Using the results of Section A3.4.5 to evaluate the derivatives in Eq. (A4.4.7), we find that

$$\partial_\tau^2 G(\chi, \tau) = v^2 f''(v\tau - |\chi|), \quad (\text{A4.4.10})$$

$$\partial_\chi G(\chi, \tau) = -\partial_\chi |\chi| f'(v\tau - |\chi|). \quad (\text{A4.4.11})$$

Differentiating Eq. (A4.4.11) by χ using $\partial_\chi^2 |\chi| = 2\delta(\chi)$ and the fact that $\delta(x)f(x) = \delta(x)f(0)$ for any function f , we find that

$$\partial_\chi^2 G(\chi, \tau) = -2\delta(\chi)f'(\nu\tau - |\chi|) + f''(\nu\tau - |\chi|). \quad (\text{A4.4.12})$$

Thus, at $\chi \neq 0$ and $\tau \neq 0$,

$$(\partial_\tau^2 - \nu^2 \partial_\chi^2)G(\chi, \tau) = 2\nu^2 \delta(\chi)f'(\nu\tau - |\chi|). \quad (\text{A4.4.13})$$

In order for $G(\chi, \tau)$ to satisfy Eq. (A4.4.6), we must have $2\nu^2 \delta(\chi)f'(\nu\tau - |\chi|) = \delta(\chi)\delta(T)$. Using $f'(\nu\tau - |\chi|) = \partial_\tau f(\nu\tau - |\chi|)/\nu$ gives

$$\partial_\tau f(\nu\tau - |\chi|) = \frac{1}{2\nu} \delta(\tau). \quad (\text{A4.4.14})$$

Using $\partial_x \Theta(x) = \delta(x)$, we find that $f(\nu\tau - \chi) = \Theta(\nu\tau - |\chi|)/2\nu$, and from Eq. (A4.4.9),

$$G(\chi, \tau) = \frac{1}{2\nu} \Theta(\nu\tau - |\chi|), \quad (\text{A4.4.15a})$$

$$G(x - x', t - t') = \frac{1}{2\nu} \Theta(\nu[t - t'] - |x - x'|). \quad (\text{A4.4.15b})$$

Equation (A4.4.15) expresses the fact that excitation from a point source at (x', t') takes time $\Delta t = |x - x'|/\nu$ to arrive at (x, t) .

Devil in the details

Although $\Theta(\nu t - |x|)$ and $\Theta(t - |x|/\nu)$ are equivalent in numerical computations, when derivatives are taken, this not the case. For example,

$$\partial_t \Theta(\nu t - |x|) = \nu \delta(\nu t - |x|), \quad (\text{A4.4.16})$$

but

$$\begin{aligned} \partial_t \Theta(t - |x|/\nu) &= \delta(t - |x|/\nu) \\ &= \frac{1}{|\nu|} \delta(\nu t - |x|). \end{aligned} \quad (\text{A4.4.17})$$

From these considerations, it is easy to show that alternative forms of the Green's function given in Eq. (A4.4.16) are

$$G(x - x', t - t') = \frac{\nu}{2} \Theta([t - t'] - |x - x'|/\nu), \quad (\text{A4.4.18a})$$

$$G(x - x', t - t') = \frac{1}{2k\omega} \Theta(\omega[t - t'] - k|x - x'|), \quad (\text{A4.4.18b})$$

where $\omega = \nu k$.

Verification

It is an interesting exercise to verify that Eq. (A4.4.15) is indeed the Green's function by substituting it into Eq. (A4.4.6). First, compute

$$\partial_t \Theta(vt - |x|) = v\delta(vt - |x|), \quad (\text{A4.4.19a})$$

which implies that

$$\partial_t^2 \Theta(vt - |x|) = v^2 \delta'(vt - |x|), \quad (\text{A4.4.19b})$$

and

$$\partial_x \Theta(vt - |x|) = -\delta(vt - |x|) \partial_x |x|, \quad (\text{A4.4.20a})$$

which implies that

$$\partial_x^2 \Theta(vt - |x|) = \delta'(vt - |x|) - 2\delta(vt - |x|)\delta(x), \quad (\text{A4.4.20b})$$

where we have used $(\partial_x |x|)^2 = 1$ and $\partial_x^2 |x| = 2\delta(x)$ (see Section A3.4.4). Substituting Eq. (A4.4.15a) into Eq. (A4.4.6) gives

$$\begin{aligned} (\partial_\tau^2 - v^2 \partial_\chi^2) G(\chi, \tau) &= v\delta(v\tau - |\chi|)\delta(\chi) \\ &= \delta(\tau - |\chi|/v)\delta(\chi). \end{aligned} \quad (\text{A4.4.21})$$

Let us now compare the integrals

$$\begin{aligned} I_1 &= \int_{-\infty}^{\infty} dx \delta(x) \int_{-\infty}^{\infty} dt \delta(t - |x|/v) f(x, t) \\ &= \int_{-\infty}^{\infty} dx \delta(x) f(x, |x|/v) \\ &= f(0, 0), \end{aligned} \quad (\text{A4.4.22})$$

and

$$\begin{aligned} I_2 &= \int_{-\infty}^{\infty} dx \delta(x) \int_{-\infty}^{\infty} dt \delta(t) f(x, t) \\ &= \int_{-\infty}^{\infty} dx \delta(x) f(x, 0) \\ &= f(0, 0). \end{aligned} \quad (\text{A4.4.23})$$

Since both $v\delta(vt - |x|)\delta(x)$ and $\delta(t)\delta(x)$ vanish at $(x, t) \neq (0, 0)$, and $I_1 = I_2$, we conclude that

$$v\delta(vt - |x|)\delta(x) = \delta(x)\delta(t), \quad (\text{A4.4.24})$$

and hence that Eq. (A4.4.15) is the correct Green's function in a unbounded 1D space.

A4.4.2 Green's function in a reflecting cavity

We now derive the Green's function needed to solve the wave equation with a source enclosed in a cavity ($0 \leq x \leq a$) with reflecting walls [Eq. (A4.4.1)]. The boundary conditions are

$$\psi(0, t) = 0, \quad (\text{A4.4.25a})$$

$$\psi(a, t) = 0. \quad (\text{A4.4.25b})$$

Assuming that $\psi = 0$ before the source turns on at $t = 0$ gives the initial conditions

$$\psi(x, 0) = 0, \quad (\text{A4.4.26a})$$

$$\partial_t \psi(x, 0) = 0. \quad (\text{A4.4.26b})$$

The Green's function for this problem must satisfy Eq. (A4.4.2) together with the boundary conditions given by Eq. (A4.4.25) and the initial conditions given by Eq. (A4.4.26).

In Section 4.1.3, separation of variables for the homogeneous wave equation gave the SHO equation

$$\left(\frac{d^2}{dt^2} + \omega^2\right)\psi(t) = 0 \quad (\text{A4.4.27})$$

with the initial condition

$$\psi(0) = \frac{d}{dt}\psi(t)\Big|_{t=0} = 0 \quad (\text{A4.4.28})$$

and the 1D Helmholtz equation

$$\left(\frac{d^2}{dx^2} + k^2\right)\psi(x) = 0. \quad (\text{A4.4.29})$$

with the boundary conditions

$$\begin{aligned} \psi(0) &= 0, \\ \psi(a) &= 0. \end{aligned} \quad (\text{A4.4.30})$$

We now conjecture that the Green's function for the wave equation in a cavity is related to the Green's function for the SHO and Green's function for the Helmholtz equation.

Green's function for the inhomogeneous Helmholtz equation

The Green's function satisfies

$$(\partial_x^2 + k^2)G(x, x') = \delta(x - x') \quad (\text{A4.4.31})$$

and the boundary conditions

$$G(x, x') = \partial_x G(x, x')|_{x=a} = 0. \quad (\text{A4.4.32})$$

Note A4.4.1

Here we do not postulate that $G(x, x') = G(x - x')$ because G is not necessarily symmetric about the source point at x' , which can be anywhere within the cavity.

Expanding the δ function in terms of the solutions of Eq. (A4.4.30) that satisfy the boundary conditions given in Eq. (A4.4.31) (see Appendix 3.4.3)

$$\delta(x - x') = \frac{2}{a} \sum_{n=1}^{\infty} \sin(k_n x) \sin(k_n x'), \quad (\text{A4.4.33})$$

we postulate a solution of the form

$$G(x, x') = \frac{2}{a} \sum_{n=1}^{\infty} c_n(x') \sin(k_n x). \quad (\text{A4.4.34})$$

Substituting Eqs. (A4.4.35) and (A4.4.34) into Eq. (A4.4.32), we obtain

$$(k^2 - k_n^2)c_n(x') = \sin(k_n x'). \quad (\text{A4.4.35})$$

Hence, the Green's function for the inhomogeneous Helmholtz equation is

$$\begin{aligned} G_H(x, x') &= \frac{2}{a} \sum_{n=1}^{\infty} \frac{\sin(k_n x) \sin(k_n x')}{k^2 - k_n^2} \\ &= \frac{1}{a} \sum_{n=1}^{\infty} \frac{\cos[k_n(x - x')] - \cos[k_n(x + x')]}{k^2 - k_n^2}. \end{aligned} \quad (\text{A4.4.36})$$

Green's function for the wave equation

Inspired by the Green's function for the SHO [Eq. (A3.3.13)] and by the Green's function for the Helmholtz equation [Eq. (A4.4.34)], we postulate the Green's function for the inhomogeneous wave equation in a cavity to be

$$G(x, t; x', t') = \Theta(t - t') \frac{2}{a} \sum_{n=1}^{\infty} c_n \frac{1}{\omega_n} \sin[\omega_n(t - t')] \sin(k_n x) \sin(k_n x'), \quad (\text{A4.4.37})$$

where $\omega_n = \nu k_n$, and the c_n values are to be determined. Substituting Eq. (A4.4.38) into Eq. (A4.4.2), and using expansion Eq. (A4.4.34) for $\delta(x - x')$, we have

$$\begin{aligned} (\partial_t^2 - \nu^2 \partial_x^2) \Theta(t - t') \frac{2}{a} \sum_{n=1}^{\infty} c_n \frac{1}{\omega_n} \sin[\omega_n(t - t')] \sin(k_n x) \sin(k_n x') \\ = \delta(t - t') \frac{2}{a} \sum_{n=1}^{\infty} \sin(k_n x) \sin(k_n x'). \end{aligned} \quad (\text{A4.4.38})$$

Evaluating the right side, and using the fact that G_{SHO} is the solution of Eq. (A3.3.2) so that

$$\partial_t^2 \left[\Theta(t - t') \frac{\sin[\omega_n(t - t')]}{\omega_n} \right] = \delta(t - t') - \omega_n \Theta(t - t') \sin[\omega_n(t - t')], \quad (\text{A4.4.39})$$

then equating the coefficients of $\sin(k_n x)$, we obtain $c_n = 1$. Thus, $G(x, t; x', t') = G(x, x'; t - t')$, and

$$G(x, x', t - t') = \Theta(t - t') \frac{2}{a} \sum_{n=1}^{\infty} \frac{1}{\omega_n} \sin[\omega_n(t - t')] \sin(k_n x') \sin(k_n x). \quad (\text{A4.4.40})$$

Using the identities

$$2 \sin a \sin b = \cos(a - b) - \cos(a + b),$$

$$2 \sin a \cos b = \sin(a + b) + \sin(a - b),$$

it can be shown that G is a superposition of a wave propagating in the $\pm x$ directions.

A4.4.3 Green's function for the unbounded damped wave equation

We need to solve

$$(\partial_t^2 + 2\alpha \partial_t - \nu^2 \partial_x^2) G(x - x', t - t') = \delta(x - x') \delta(t - t'). \quad (\text{A4.4.41})$$

This is an unexpectedly difficult problem because there is no general solution of the damped wave equation analogous to the form of Eq. (A4.4.8).

References

1. E. I. Butikov, “Misconceptions about the energy of waves in a strained string,” *Physica Scripta* **86**, 035403 (2012).
2. L. M. Burko, “Energy in one-dimensional linear waves in a string,” *arXiv:1007.3962* [physics.class-ph] (2010).

Chapter 5

FDTD Algorithms for the 1D Equation

In Chapter 3 we developed the basic concepts of standard and nonstandard finite difference models with respect to the simple harmonic oscillator. We now extend these developments to the next level of complexity, the 1D wave equation, and thereby set the stage to deal with the 2D and 3D wave equations and with Maxwell's equations.

FDTD algorithms to solve the 1D wave equation may seem simple, but in fact there are many 'devils in the details' that must be smitten before FDTD can be used to solve interesting problems. Dealing with these 'devils' in one dimension will make it easier to handle them later on in two and three.

Topics:

- Standard and nonstandard FDTD for the wave equation in different forms
- Accuracy and stability
- Other constraints

5.1 Homogeneous Wave Equation

5.1.1 Standard finite difference model

As usual, d_x and d_t denote central finite difference operators unless otherwise specified. Inserting the FD expressions for derivatives $\partial_t^2 \rightarrow d_t^2/\Delta t^2$ and $\partial_x^2 \rightarrow d_x^2/\Delta x^2$ (see Chapter 1) into the wave equation,

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = 0, \quad (5.1)$$

we obtain its second-order standard finite difference (S-FD) model,

$$\left(d_t^2 - \frac{v^2 \Delta t^2}{\Delta x^2} d_x^2 \right) \psi(x, t) = 0. \quad (5.2)$$

Expanding $d_t^2\psi(x, t) = \psi(x, t + \Delta t) + \psi(x, t - \Delta t) - 2\psi(x, t)$ and solving for $\psi(x, t + \Delta t)$ yields what we call the standard (S) FDTD algorithm:

$$\psi(x, t + \Delta t) = -\psi(x, t - \Delta t) + \left(2 + \frac{v^2\Delta t^2}{\Delta x^2}d_x^2\right)\psi(x, t). \quad (5.3)$$

Given $\psi(x, 0)$ and $\psi(x, \Delta t)$, we can iterate Eq. (5.3) to compute all future wave fields.

5.1.2 Error of the standard finite difference model

Letting $u = v\Delta t/\Delta x$, and inserting a general solution (see Section 4.1.1) $f(x - vt)$ into the S-FD model, we obtain

$$\begin{aligned} \left(d_t^2 - \frac{v^2\Delta t^2}{\Delta x^2}d_x^2\right)f(x - vt) &= f(x - vt + u\Delta x) + f(x - vt - u\Delta x) \\ &\quad - 2f(x - vt) - [f(x - vt + \Delta x) \\ &\quad + f(x - vt - \Delta x) - 2f(x - vt)] \\ &= -\frac{1 - u^4}{12}\Delta x^4 f^{(4)}(x - vt) + \dots \end{aligned} \quad (5.4)$$

The deviation of the right side of Eq. (5.4) from zero measures the error of the FD model.

It is interesting to note that although the S-FD approximations of the derivatives are only second-order accurate, the S-FD model of the wave equation is fourth-order accurate because the second-order errors cancel. In fact, if $u = 1$, the errors completely cancel, and Eq. (5.2) becomes an exact model of the wave equation.

Unfortunately, we cannot take $u = 1$ in most problems. Usually, we want to solve problems with interfaces between different media for which the wave equation takes the form

$$\left(\partial_t^2 - \frac{v_0^2}{n^2}\partial_x^2\right)\psi(x, t) = 0, \quad (5.5)$$

where the index of refraction n (and hence $v = v_0/n$) is a function of position. One might try to maintain $u = 1$ by varying Δx , but across interfaces of different Δx , the error of the central FD expressions rises from second-order to first-order, and the errors fail to cancel.

Unless otherwise specified, we assume a uniform space–time grid with constant values for Δx and Δt .

5.1.3 Nonstandard finite difference model

Putting u in place of $v\Delta t/\Delta x$ in model Eq. (5.2) and inserting the monochromatic solution $\varphi = e^{i(kx-\omega t)}$, we obtain

$$\begin{aligned}(d_t^2 - u^2 d_x^2)\varphi &= 4[-\sin^2(\omega \Delta t/2) + u^2 \sin^2(k \Delta x/2)]\varphi \\ &= \varepsilon \varphi,\end{aligned}\tag{5.6}$$

where $v = \omega/k = v_0$. The quantity ε is a measure of the error of the FD model. For $u = v\Delta t/\Delta x \neq 1$, $\varepsilon \neq 0$ so φ is not a solution of the wave equation model [Eq. (5.2)]. However, the error can be made to vanish by choosing $u = \tilde{v}$, where

$$\tilde{v} = \frac{\sin(\omega \Delta t/2)}{\sin(k \Delta x/2)},\tag{5.7}$$

where $\tilde{v}$ is the effective propagation velocity on the grid. With this choice, $\varepsilon = 0$, and φ is a solution of both the wave equation and what we call its nonstandard (NS) FD model:

$$(d_t^2 - \tilde{v}^2 d_x^2)\psi(x, t) = 0.\tag{5.8}$$

We now construct a NS-FD model of Eq. (5.5), which includes the refractive index. Expressing $\tilde{v}$ in the form

$$\tilde{v} = \frac{\tilde{v}_0}{\tilde{n}},\tag{5.9}$$

where

$$\tilde{v}_0 = \frac{\sin(\omega \Delta t/2)}{\sin(k_0 \Delta x/2)},\tag{5.10}$$

and

$$\tilde{n} = \frac{\sin(n k_0 \Delta x/2)}{\sin(k_0 \Delta x/2)}\tag{5.11}$$

is the effective index of refraction on the grid, the NS-FD model of the wave equation [Eq. (5.5)] becomes

$$\left(d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} d_x^2\right)\psi(x, t) = 0.\tag{5.12}$$

Now $\varphi = e^{i(n k_0 x - \omega t)}$ is a solution of both the wave equation and its NS-FD model [Eq. (5.12)] in each region of constant n . A nearly exact NS-FDTD algorithm is thus

$$\psi(x, t + \Delta t) = -\psi(x, t - \Delta t) + \left(2 + \frac{\tilde{v}_0^2}{\tilde{n}^2} d_x^2\right) \psi(x, t). \quad (5.13)$$

Across interfaces between regions of different n , accuracy falls, but numerical experiments show that the NS-FDTD algorithm is still much more accurate than the S-FDTD algorithm.

Note 5.1

For all ω and k that satisfy Eq. (5.7), the error of the NS-FDTD algorithm vanishes as long as $\omega\Delta t$ and $k\Delta t$ satisfy the Nyquist limit (see Section 5.1.4); thus, using NS-FDTD it is possible to simultaneously compute wave propagation with multiple frequencies. In spectrum calculations, however, when there are different materials, some error arises—especially over a broad band—because the effective index of refraction varies slightly with frequency. This error can be reduced by an interpolation procedure that is explained in Section 6.5.4.

5.1.4 Devil in the details

Simple though they might seem, actually using the FDTD algorithms just introduced to solve real problems is far from trivial. With respect to a wave of wavelength λ and period T , the three most important parameters are the ratios $\lambda/\Delta x$, $T/\Delta t$, and $u = v\Delta t/\Delta x$.

Nyquist limit

In accord with the Nyquist limit,¹ Δx and Δt are constrained by

$$\lambda/\Delta x > 2, \quad (5.14a)$$

and

$$T/\Delta t > 2. \quad (5.14b)$$

In order to represent both the amplitude and phase of a harmonic signal on a periodic grid, more than two samples per period are required (see Fig. 5.1). If the wave is a superposition of many monochromatic waves, then Eq. (5.14) applies to the shortest wavelength and shortest period.

The error of the S-FD model for $u < 1$ depends on the ratio $\lambda/\Delta x$; the shorter the wavelength the larger the error. Thus, when a polychromatic wave is propagated on the numerical grid using S-FDTD, different wavelength components have different errors.

Numerical stability

In addition to the constraints given in Eq. (5.14), Δx and Δt must be chosen such that

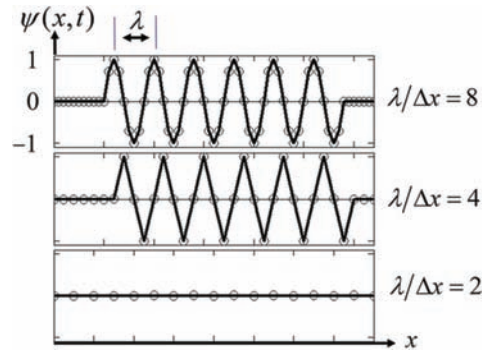


Figure 5.1 Representation of $\psi(x, t)$ at a fixed time for different discretizations ($\lambda/\Delta x$).

$$\frac{v\Delta t}{\Delta x} \leq 1 \quad (5.15)$$

in order to maintain algorithm stability (see Appendix 7.1), where v is the greatest velocity in the computation. Since $v = \lambda/T$, we must always choose $T/\Delta t \geq \lambda/\Delta x$.

Iteration

To iterate the FDTD algorithm, it is necessary to input the two initial fields, $\psi(x, 0)$ and $\psi(x, \Delta t)$, but these fields may not always be known. This difficulty can be circumvented by letting $\psi(x, -\Delta t) = \psi(x, 0) = 0$ and using a source to generate the input fields (see Section 5.3).

5.1.5 Precursor waves: physical insights

A good model not only explains the phenomena it was designed to explain, but also predicts new phenomena yet to be observed. Let $v\Delta t/\Delta x = 1/2$, and let a wavefront be located at $x = 0$ at time $t = 0$. Then, at $t = \Delta t$ the wavefront ought to advance by $\Delta x/2$, but it cannot because the field is not computed between the grid points. But some small amount of “precursor” excitation reaches $x = \Delta x$ at $t = \Delta t$, while the main wavefront arrives at $x = \Delta x$ at $t = 2\Delta t$. Regardless of the value of $v\Delta t/\Delta x < 1$ in the FDTD algorithm, some small precursor excitation travels as if $v\Delta t/\Delta x = 1$.

In Fig. 5.2, a sinusoidal source is turned on at $x = 0$ and $t = 0$ with $v\Delta t/\Delta x = 1/2$. At $t = 3T$ (T is the wave period), the main wavefront has advanced to $x = \pm 3\lambda$ (λ , the wavelength, is an integer number of grid spaces) from the source, but the leading edge of the precursor field p has reached $x = \pm 6\lambda$. In the figure, p is transformed and scaled up for visibility. The precursor constitutes a source of computational “noise” that can give rise to error and numerical instability in FDTD calculations.

The precursor can be understood mathematically by examining the discrete Green’s function (see Appendix 6.1) for $u = 1/2$. The main wave

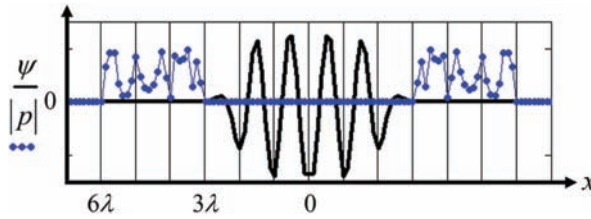


Figure 5.2 Main wave ψ and its precursor p at $t = 3T$ due to a sinusoidal source turned on at $x = 0$ and $t = 0$. In the interval $6\lambda < |x| < 3\lambda$, $10^{-15} < |p| < 10^{-3}$. $|p|$ (transformed and scaled for visibility) falls off approximately exponentially with distance from the source.

envelope has a half-width of $ut = t/2$ but is nonzero up to a distance of t grid spacings on either side of the source, as if $v\Delta t/\Delta x = 1$.

The FDTD precursor wave has a physical analog. If light impinges onto (for example) a 3-m-thick material with a refractive index of 3, then we expect that a signal should appear on the opposite face after 30 ns, but in fact a small amplitude signal can be experimentally observed after just 10 ns, as if the light were traveling with its vacuum velocity through the material. The physical precursor is a consequence of dispersion and is more thoroughly analyzed in Ref. 2.

The 1D stability limit [Eq. (5.15)] can be understood heuristically from the fact that each nonzero field point on the spatial grid acts as a source (Huygens' model on a grid), and at the next time step it can excite only its nearest neighbors, but no others. Thus in FDTD, an excitation can travel only one space step in one time step, regardless of the value of $v\Delta t/\Delta x$.

The finite speed of light is a physical phenomenon, yet it comes naturally out of FDTD. As we shall see in two and three dimensions (in Appendix 7.1), the speed of propagation on the spatial grid also depends on its dimensionality and connectivity. This leads one to speculate that the speed of light depends on the geometry of space-time.

5.2 Damped Wave Equation

The damped wave equation (see Section 4.3.2) is

$$\left(\partial_t^2 + 2\alpha\partial_t - v^2\partial_x^2\right)\psi(x, t) = 0. \quad (5.16)$$

5.2.1 Standard finite difference models

Following Section 3.6, the first-order time derivative can be modeled either by the standard forward finite difference (SF-FD) expression

$$\partial_t\psi(x, t) \cong \frac{\psi(x, t + \Delta t) - \psi(x, t)}{\Delta t}, \quad (5.17a)$$

by the standard backward (SB-FD) expression

$$\partial_t \psi(x, t) \cong \frac{\psi(x, t) - \psi(x, t - \Delta t)}{\Delta t}, \quad (5.17b)$$

or by the double-step standard central finite difference (SC-FD) approximation

$$\partial_t \psi(x, t) \cong \frac{\psi(x, t + \Delta t) - \psi(x, t - \Delta t)}{2\Delta t}. \quad (5.17c)$$

The second-order derivatives are modeled by $\partial_t^2 \cong d_t^2/\Delta t^2$ and $\partial_x^2 \cong d_x^2/\Delta x^2$. The different S-FD models are given below:

SF-FD model:

$$d_\tau^2 \psi_\chi^\tau + 2\alpha \Delta t \left(\psi_\chi^{\tau+1} - \psi_\chi^\tau \right) - \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \psi_\chi^\tau = 0, \quad (5.18a)$$

$$\psi_\chi^{\tau+1} + \frac{1}{1 + 2\alpha \Delta t} \left\{ \psi_\chi^{\tau-1} - \left[2(1 + \alpha \Delta t) + \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right] \psi_\chi^\tau \right\} = 0, \quad (5.18b)$$

SB-FD model:

$$d_\tau^2 \psi_\chi^\tau + 2\alpha \Delta t \left(\psi_\chi^\tau - \psi_\chi^{\tau-1} \right) - \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \psi_\chi^\tau = 0, \quad (5.19a)$$

$$\psi_\chi^{\tau+1} + (1 - 2\alpha \Delta t) \psi_\chi^{\tau-1} - \left[2(1 - \alpha \Delta t) + \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right] \psi_\chi^\tau = 0, \quad (5.19b)$$

SC-FD model:

$$d_\tau^2 \psi_\chi^\tau + \alpha \Delta t \left(\psi_\chi^{\tau+1} - \psi_\chi^{\tau-1} \right) - \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \psi_\chi^\tau = 0, \quad (5.20a)$$

$$\psi_\chi^{\tau+1} + \frac{1 - \alpha \Delta t}{1 + \alpha \Delta t} \psi_\chi^{\tau-1} - \frac{1}{1 + \alpha \Delta t} \left(2 + \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right) \psi_\chi^\tau = 0. \quad (5.20b)$$

Note 5.2

While the S-FD model of the lossless wave equation is exact for $\nu \Delta t / \Delta x = 1$, for the lossy wave equation none of the above S-FD models is exact, even for $\nu \Delta t / \Delta x = 1$.

The corresponding FDTD algorithms become:

SF-FDTD:

$$\psi_\chi^{\tau+1} = \frac{1}{1 + 2\alpha \Delta t} \left\{ -\psi_\chi^{\tau-1} + \left[2(1 + \alpha \Delta t) + \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right] \psi_\chi^\tau \right\}, \quad (5.21)$$

SB-FDTD:

$$\psi_{\chi}^{\tau+1} = -(1 - 2\alpha\Delta t)\psi_{\chi}^{\tau-1} + \left[2(1 - \alpha\Delta t) + \frac{v^2\Delta t^2}{\Delta x^2}d_{\chi}^2\right]\psi_{\chi}^{\tau}, \quad (5.22)$$

SC-FDTD:

$$\psi_{\chi}^{\tau+1} = -\left(\frac{1 - \alpha\Delta t}{1 + \alpha\Delta t}\right)\psi_{\chi}^{\tau-1} + \frac{1}{1 + \alpha\Delta t}\left(2 + \frac{v^2\Delta t^2}{\Delta x^2}d_{\chi}^2\right)\psi_{\chi}^{\tau}. \quad (5.23)$$

Note 5.3

The stability condition for SB-FD is $\nu\Delta t/\Delta x < 1$. It is numerically unstable at $\nu\Delta t/\Delta x = 1$. SF- and SC-FDTD are numerically stable for $\nu\Delta t/\Delta x \leq 1$.

Let us define the solution error ε by $W(\psi) = \varepsilon\psi$, where W denotes the operation on the left side of Eqs. (5.18a), (5.19a), or (5.20a), and ψ is the complex-wavenumber solution (see Section 4.2). We do not examine the complex-frequency solution because it is irrelevant for our purposes. The analytical error analysis for these FD models is tedious, so we omit it here, but from numerical calculations for typical FDTD parameters, we find that the error of the SC-FD model is the lowest, and the error of SF-FD model is the highest—much higher than that of the SB-FD model. These calculations are given in Program MC5.1.

5.2.2 Nonstandard finite difference models

We now proceed to develop a nonstandard finite difference (NS-FD) model and a nonstandard finite difference time domain (NS-FDTD) algorithm with respect to the complex wavenumber solution of the damped wave equation.

Inserting the substitutions $\nu\Delta t/\Delta x \rightarrow \tilde{\nu}_f$ and $\alpha\Delta t \rightarrow \tilde{\alpha}_f$ into Eq. (5.18a), $\nu\Delta t/\Delta x \rightarrow \tilde{\nu}_b$ and $\alpha\Delta t \rightarrow \tilde{\alpha}_b$ into Eq. (5.19a), and $\nu\Delta t/\Delta x \rightarrow \tilde{\nu}_c$ and $\alpha\Delta t \rightarrow \tilde{\alpha}_c$ into Eq. (5.20a), respectively, we obtain the nonstandard forward (NSF), nonstandard backward (NSB), and nonstandard central (NSC) finite difference models given below:

NSF-FD model:

$$d_{\tau}^2\psi_{\chi}^{\tau} + 2\tilde{\alpha}_f(\psi_{\chi}^{\tau+1} - \psi_{\chi}^{\tau}) - \tilde{\nu}_f^2 d_{\chi}^2\psi_{\chi}^{\tau} = 0, \quad (5.24)$$

NSB-FD model:

$$d_{\tau}^2\psi_{\chi}^{\tau} + 2\tilde{\alpha}_b(\psi_{\chi}^{\tau} - \psi_{\chi}^{\tau-1}) - \tilde{\nu}_b^2 d_{\chi}^2\psi_{\chi}^{\tau} = 0, \quad (5.25)$$

NSC-FD model:

$$d_\tau^2 \psi_\chi^\tau + \tilde{\alpha}' (\psi_\chi^{\tau+1} - \psi_\chi^{\tau-1}) - \tilde{\nu}^2 d_\chi^2 \psi_\chi^\tau = 0. \quad (5.26)$$

With the appropriate choice of parameters, all of the models can be made to be exact with respect to the analytic solution of the damped wave equation, regardless of how the $\partial_t \psi$ term is modeled, and they all reduce to the common exact NS-FD model:

$$\psi_\chi^{\tau+1} - B\psi_\chi^\tau + C\psi_\chi^{\tau-1} = 0. \quad (5.27)$$

Mathematically, it is easiest to derive the NS-FD parameters using the NSC-FD model. Inserting an analytical complex wavenumber solution of the damped wave equation,

$$\psi(x, t) = e^{i(\omega t - k' x)}, \quad (5.28)$$

where $k' = k\sqrt{1 - 2i\alpha/\omega} = k_r' + ik_i'$, into the NSC-FD model [Eq. (5.26)], we obtain

$$-4\sin^2(\omega \Delta t/2) + 2i\tilde{\alpha}' \sin(\omega \Delta t) + 4\tilde{\nu}^2 \sin^2(k' \Delta x/2) = 0. \quad (5.29)$$

Using the identities $2\sin^2(x/2) = 1 - \cos x$, $\cos(x + iy) = \cos x \cosh y - i \sin x \sinh y$, and equating the real and imaginary parts of Eq. (5.29) to zero, we find that

$$\tilde{\nu}^2 = \frac{2\sin^2(\omega \Delta t/2)}{1 - \cos(k_r' \Delta x) \cosh(k_i' \Delta x)}, \quad (5.30a)$$

$$\begin{aligned} \tilde{\alpha}' &= \frac{-\tilde{\nu}^2 \sin(k_r' \Delta x) \sinh(k_i' \Delta x)}{\sin(\omega \Delta t)} \\ &= -\tan(\omega \Delta t/2) \frac{\sin(k_r' \Delta x) \sinh(k_i' \Delta x)}{1 - \cos(k_r' \Delta x) \cosh(k_i' \Delta x)}. \end{aligned} \quad (5.30b)$$

An exact FD model of the damped wave equation with respect to the complex wavenumber solution is thus

$$d_\tau^2 \psi_\chi^\tau + \tilde{\alpha}' (\psi_\chi^{\tau+1} - \psi_\chi^{\tau-1}) - \tilde{\nu}^2 d_\chi^2 \psi_\chi^\tau = 0. \quad (5.31)$$

Regardless of how the $\partial_t \psi$ term is modeled, an exact NS-FDTD algorithm is

$$\psi_\chi^{\tau+1} = \frac{1}{1 + \tilde{\alpha}'} \left[-(1 - \tilde{\alpha}') \psi_\chi^{\tau-1} + 2\psi_\chi^\tau + \tilde{\nu}^2 d_\chi^2 \psi_\chi^\tau \right]. \quad (5.32)$$

5.3 Wave Equation with a Source

5.3.1 Standard finite difference model: lossless case

The wave equation with a source is

$$\left(\partial_t^2 - v^2 \partial_x^2\right) \psi(x, t) = s(x, t). \quad (5.33)$$

Substituting S-FD expressions for the derivatives, we obtain the S-FD model

$$\left(d_t^2 - \frac{v^2 \Delta t^2}{\Delta x^2} d_x^2\right) \psi(x, t) = \Delta t^2 s(x, t) \quad (5.34)$$

and the corresponding S-FDTD algorithm

$$\psi_x^{\tau+1} = -\psi_x^{\tau-1} + \left(2 + \frac{v^2 \Delta t^2}{\Delta x^2} d_x^2 \psi_x^\tau\right) + \Delta t^2 s_x^\tau. \quad (5.35)$$

Note 5.4

Even when $v\Delta t/\Delta x = 1$, the S-FD model is not exact.

As an example, we now construct a S-FD model of the wave equation with a harmonic point source given by $s(x, t) = \delta(x)\Theta(t)e^{i\omega t}$. Modeling $\delta(x)$ by

$$\delta(x) \cong \frac{\delta_{x,0}}{\Delta x}, \quad (5.36)$$

where $\delta_{x,0} = 1$ for $x = 0$, and $\delta_{x,0} = 0$ for $x \neq 0$, the FD model of the wave equation with $s(x, t) = \delta(x)\Theta(t)e^{i\omega t}$ becomes

$$\left(d_t^2 - \frac{v^2 \Delta t^2}{\Delta x^2} d_x^2\right) \psi(x, t) = \frac{\Delta t^2}{\Delta x} \delta_{x,0} \Theta(t) e^{i\omega t}. \quad (5.37)$$

The S-FDTD algorithm is thus

$$\psi_x^{\tau+1} = -\psi_x^{\tau-1} + \left(2 + \frac{v^2 \Delta t^2}{\Delta x^2} d_x^2 \psi_x^\tau\right) + \frac{\Delta t^2}{\Delta x} \delta_{x,0} \Theta(\tau) e^{i\omega \tau \Delta t} \quad (5.38)$$

with the initial conditions $\psi_x^{-1} = \psi_x^0 = 0$. Thus, in the S-FD model, a unit source has amplitude $\Delta t/\Delta x^2$.

5.3.2 Standard finite difference model: damped case

For the damped wave equation with a source

$$\left(\partial_t^2 + 2\alpha \partial_t - v^2 \partial_x^2\right) \psi(x, t) = s(x, t), \quad (5.39)$$

the three possible S-FD models and their corresponding S-FDTD algorithms are as follows:

SF-FD model and SF-FDTD:

$$d_\tau^2 \psi_\chi^\tau + 2\alpha\Delta t \left(\psi_\chi^{\tau+1} - \psi_\chi^\tau \right) - \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \psi_\chi^\tau = \Delta t^2 s_\chi^\tau, \quad (5.40)$$

$$\psi_\chi^{\tau+1} = \frac{1}{1 + 2\alpha\Delta t} \left\{ \left[2(1 + \alpha\Delta t) + \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right] \psi_\chi^\tau + \Delta t^2 s_\chi^\tau \right\}, \quad (5.41)$$

SB-FD model and SB-FDTD:

$$d_\tau^2 \psi_\chi^\tau + 2\alpha\Delta t \left(\psi_\chi^\tau - \psi_\chi^{\tau-1} \right) - \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \psi_\chi^\tau = \Delta t^2 s_\chi^\tau, \quad (5.42)$$

$$\psi_\chi^{\tau+1} = -(1 - 2\alpha\Delta t) \psi_\chi^{\tau-1} + \left[2(1 - \alpha\Delta t) + \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right] \psi_\chi^\tau + \Delta t^2 s_\chi^\tau, \quad (5.43)$$

SC-FD model and SC-FDTD:

$$d_\tau^2 \psi_\chi^\tau + \alpha\Delta t \left(\psi_\chi^{\tau+1} - \psi_\chi^{\tau-1} \right) - \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \psi_\chi^\tau = \Delta t^2 s_\chi^\tau, \quad (5.44)$$

$$\psi_\chi^{\tau+1} = -\left(\frac{1 - \alpha\Delta t}{1 + \alpha\Delta t} \right) \psi_\chi^{\tau-1} + \frac{1}{1 + \alpha\Delta t} \left(2 + \frac{v^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right) \psi_\chi^\tau + \frac{\Delta t^2 s_\chi^\tau}{1 + \alpha\Delta t}. \quad (5.45)$$

5.3.3 Nonstandard finite difference model: lossless case

Let us now construct an exact NS-FD model with respect to the harmonic point source, $s(x, t) = \delta(x)\Theta(t)e^{i\omega t}$. Since the NS-FD model of the homogeneous equation ($s = 0$) is exact, we postulate a model of the form

$$\left(d_t^2 - \tilde{v}^2 d_x^2 \right) \psi(x, t) = \tilde{A} \delta_{x,0} \Theta(t) e^{i\omega t}, \quad (5.46)$$

where $\tilde{v} = \sin(\omega\Delta t/2)/\sin(k\Delta x/2)$, and $\Delta t^2/\Delta x \rightarrow \tilde{A}$, the NS amplitude, which is to be determined. Inserting the analytic solution ψ_0 (see Section 4.3.1)

$$\psi_0(x, t) = \frac{1}{2iv^2k} \Theta(vt - |x|) (e^{i(\omega t - k|x|)} - 1) \quad (5.47)$$

into the model at $x = 0$ and $t > \Delta x/\nu$ (so that $\Theta(\omega t - k|x|) = 1$), and using the identities

$$d_x^2 e^{-ik|x|}|_{x=0} = 2(e^{-ik\Delta x} - 1), \quad (5.48a)$$

$$d_t^2 e^{i\omega t} / e^{i\omega t} = -4 \sin^2(\omega \Delta t / 2), \quad (5.48b)$$

and $e^{-ik\Delta x} - 1 = -2ie^{-ik\Delta x/2} \sin(k\Delta x/2)$, we have the expressions

$$(d_t^2 - \tilde{v}^2 d_x^2) \psi(x, t) = \tilde{A} \delta_{x,0} \Theta(t) e^{i\omega t}, \quad (5.49)$$

$$\left[-4 \sin^2(\omega \Delta t / 2) + 4i \frac{\sin^2(\omega \Delta t / 2)}{\sin^2(k \Delta x / 2)} e^{-ik\Delta x/2} \sin(k\Delta x/2) \right] \frac{1}{2iv^2 k} e^{i\omega t} = \tilde{A} e^{i\omega t}. \quad (5.50)$$

We find that Eq. (5.49) is an equality if

$$\tilde{A} = \frac{2 \sin^2(\omega \Delta t / 2)}{v^2 k \tan(k \Delta x / 2)}. \quad (5.51)$$

As it ought, $\tilde{A} \rightarrow \Delta t^2 / \Delta x$ in the limits $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$, but for non-infinitesimal Δx and Δt , for example, if

$$\Delta x = \lambda / 8, \quad (5.52a)$$

$$v \Delta t / \Delta x = 1, \quad (5.52b)$$

we find that the ratio of the NS amplitude to the S amplitude is $\tilde{A} / (\Delta t^2 / \Delta x) = 0.90$.

The NS-FDTD algorithm for the wave equation with a unit amplitude harmonic point source s_h of angular frequency ω located at x' is thus

$$\psi(x, t + \Delta t) = -\psi(x, t - \Delta t) + (2 + \tilde{v}^2 d_x^2) \psi(x, t) + \tilde{A} \Theta(t) s_h(t) \delta_{x,x'}. \quad (5.53)$$

Both the S- and NS-FDTD algorithms are iterated from the initial fields

$$\psi(x, 0) = 0, \quad (5.54a)$$

$$\psi(x, -\Delta t) = 0. \quad (5.54b)$$

Transient devils

For $s(x, t) = \delta(x) \Theta(t) \cos(\omega t)$ in Eq. (5.33), the analytic solution is $\psi_{\text{Re}0} = \text{Re}(\psi_0)$, where ψ_0 is given by Eq. (5.47), and

$$\psi_{\text{Re}0}(x, t) = \frac{1}{2v^2 k} \Theta(\omega t - k|x|) \sin(t - |x|/v). \quad (5.55)$$

Comparing $\psi_{\text{Re}0}$ with an NS-FDTD calculation [Fig. 5.3(a)], we find that the error is very large. This is a numerical effect caused by abruptly turning on the source, which gives rise to numerical transients. This numerical error

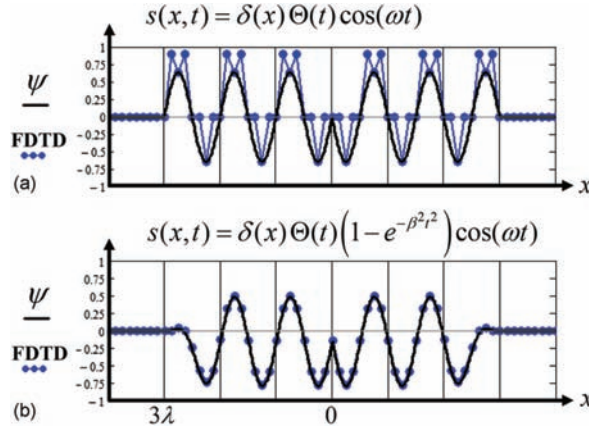


Figure 5.3 (a) NS-FDTD calculation versus (b) analytic solution for different time dependences of a point source with $\nu\Delta t/\Delta x = 1$, $\lambda/\Delta x = 8$, and $1/\beta = T/2$.

can be almost eliminated by replacing the step function with a turn-on function such as

$$\Theta_c(t) = \Theta(t)(1 - e^{-\beta t}), \quad (5.56a)$$

$$\Theta_g(t) = \Theta(t)(1 - e^{-\beta^2 t^2}), \quad (5.56b)$$

which “slowly” increases the source amplitude with a rise time of $b = 1/\beta$, where $\beta > 0$. Numerical experiments show that the calculation is insensitive to the exact value of b , but it should be on the order of one wave period. As can be seen in Fig. 5.3(b), setting $b = T/2$ in a Gaussian turn-on function reduces the error of the NS-FDTD calculation to nearly zero.

NS-FDTD with a turn-on function

Recall from Section 4.3.1 that the analytic solution of

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = \Theta(t) (1 - e^{-\beta t}) e^{i\omega t} \delta(x) \quad (5.57)$$

is

$$\psi_e(x, t) = \psi_0(x, t) - \Delta\psi_e(x, t), \quad (5.58)$$

where

$$\Delta\psi_e(x, t) = \frac{1}{2i\bar{\omega}v} \Theta(\omega t - k|x|) \left[e^{i(\omega t - \bar{k}|x|)} - 1 \right], \quad (5.59)$$

$\bar{\omega} = \omega + i\beta$, $\bar{k} = \bar{\omega}/v$, and ψ_0 is given by Eq. (5.47).

We now postulate an NS-FD model of the form

$$\left(d_t^2 - \tilde{v}^2 d_x^2\right) \psi(x, t) = \delta_{x,0} \Theta(t) (\tilde{A} e^{i\omega t} - B e^{i\omega t} e^{-\beta t}), \quad (5.60)$$

where $\tilde{A}$ is given by Eq. (5.51). Taking $\psi = \psi_e$, evaluating the right side of Eq. (5.60) at $x = 0$ for $t > \Delta x/\nu$, and solving for B , we find that

$$B = \frac{2}{\bar{\omega} \nu} \left[i \sin^2(\bar{\omega} \Delta t/2) + e^{-i\bar{k} \Delta x/2} \frac{\sin^2(\omega \Delta t/2)}{\sin^2(k \Delta x/2)} \sin(\bar{k} \Delta x/2) \right]. \quad (5.61)$$

For typical FDTD parameters such as Eq. (5.52) and $b = T$, we find that $\tilde{A} = 0.900$ and $B = 0.902 + 0.030i \cong \tilde{A}$, where T is the wave period. It is easy to show that $B = \tilde{A}$ in the limits $\lambda/\Delta x$, $T/\Delta t$, and $b \rightarrow \infty$. Thus, for typical parameters of FDTD calculations, $B \cong \tilde{A}$, and an excellent NS-FD model for a harmonic source with the turn-on function Θ_e is

$$\left(d_t^2 - u^2 d_x^2\right) \psi(x, t) = \tilde{A} \delta_{x,0} \Theta(t) (1 - e^{-\beta/t}) e^{i\omega t}. \quad (5.62)$$

Although $\Delta\psi_e$ is not an exact solution of the homogeneous wave equation, the error of the model [Eq. (5.62)] is small. For $s(x, t) = \delta(x)\Theta(t)(1 - e^{-\beta/t})\cos(\omega t)$ in Eq. (5.33), the analytic solution is $\psi_{ec} = \text{Re}(\psi_e)$. Similar considerations apply for the Gaussian turn-on function $\Theta_g(t)$, and $\tilde{A}$ is again the correct amplitude as shown in Fig. 5.3(b). In Fig. 5.4 we plot the deviation of the NS- and S-FDTD calculations from the analytic solution for the exponential turn-on function for the parameter [Eq. (5.52)] and $b = T$. The root-mean-square deviation of ψ_{NS} from the analytic solution is $\delta_{NS} = 0.016$, and that of ψ_S is $\delta_S = 0.036$. In Fig. 5.5 we plot the deviations $\Delta\psi_{NS}$ and $\Delta\psi_S$ from the analytic solution for a point cosine source with a Gaussian turn-on function using $\Delta x = \lambda/8$, $\nu\Delta t/\Delta x = 2/3$, and $b = T/2$. Most of the error arises when the source turns on and can be reduced by using a longer rise time. Comparing Figs. 5.4 and 5.5 we see that, except at the leading edge of the

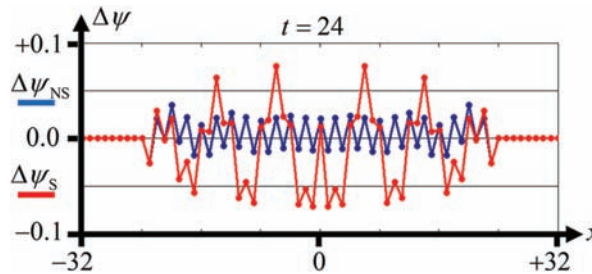


Figure 5.4 Deviation of the NS- and S-FDTD calculations from the analytic solution for an exponential turn-on function with $\delta_{NS} = 0.016$, $\delta_S = 0.036$, $\Delta x = \lambda/8$, $\nu\Delta t/\Delta x = 1$, and $1/\beta = T$.

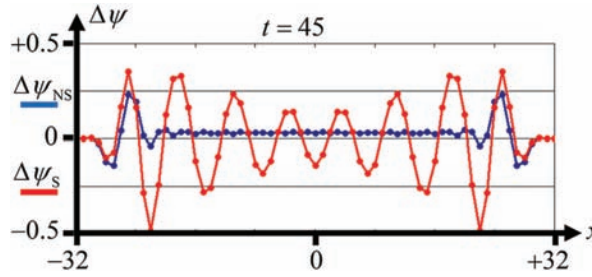


Figure 5.5 Deviation of the NS- and S-FDTD calculations from the analytic solution for a Gaussian turn-on function with $\delta_{NS} = 0.068$, $\delta_S = 0.195$, $\Delta x = \lambda/8$, $\nu\Delta t/\Delta x = 2/3$, and $b = T/2$.

wave front, the error is lower for $\nu\Delta t/\Delta x = 2/3$ than for $\nu\Delta t/\Delta x = 1$. See Appendix 4.1 for a discussion.

5.3.4 Nonstandard finite difference model: damped case

Following Section 5.3.3, we now develop the NS-FDTD algorithm for a point harmonic source in a lossy medium. We model

$$\left(\partial_t^2 + 2\alpha\partial_t - \nu^2\partial_x^2\right)\psi(x, t) = \Theta(t)\delta(x) e^{i\omega t} \quad (5.63)$$

by

$$d_\tau^2\psi_\chi^\tau + \tilde{\alpha}'\left(\psi_\chi^{\tau+1} - \psi_\chi^{\tau-1}\right) - \tilde{\nu}'^2 d_\chi^2\psi_\chi^\tau = \tilde{A}' \Theta(t)\delta_{x,0} e^{i\omega t}, \quad (5.64)$$

where $\tilde{A}'$ is the nonstandard source amplitude, which is to be determined. This model is exact for $x \neq 0$. We now require that the solution of the differential [Eq. (5.63)], given by (see Section 4.3.2)

$$\psi_0(x, t) = \frac{1}{2i\nu^2 k'} \Theta(\nu t - |x|) e^{i(\omega t - k'|x|)}, \quad (5.65)$$

also be a solution of difference Eq. (5.64). Evaluating the solution [Eq. (5.65)] at $x = 0$ and $t > \Delta x/\nu$, and using the identity [Eq. (5.48)], we find that

$$\tilde{A}' = \left(\frac{\sin k'}{\nu^2 k'}\right) \left[\frac{2 \sin^2(\omega\Delta t/2)}{1 - \cos k'_r \cosh k'_i}\right]. \quad (5.66)$$

As $\alpha \rightarrow 0$, $k' \rightarrow k$, and, as expected, $\tilde{A}' \rightarrow \tilde{A}$. The fact that $\tilde{A}'$ is complex means that the real and imaginary parts of the source mix. Writing $\tilde{A}' = |\tilde{A}'|e^{i\phi_{NS}}$, the NS model of a unit amplitude harmonic source $e^{i\omega t}$ is $\tilde{A}'e^{i\omega t} = |\tilde{A}'|e^{i(\omega t + \phi_{NS})}$. Taking $\Delta x = \lambda/8$, $\nu\Delta t/\Delta x = 1/2$, and $\alpha = \omega/8$, which implies that $k\Delta x = \pi/4$, and $\Delta t = T/16$, which implies that $\omega\Delta t = \pi/8$, we find that

$$\tilde{A}' \cong 0.933 + 0.025i. \quad (5.67)$$

Keeping the other parameters constant and taking $\alpha = \omega/16$, we find that $\tilde{A}' \cong 0.936 + 0.006i$. The imaginary part decreases with falling α and rising $\nu\Delta t/\Delta x$. For most calculations, we can thus neglect the imaginary part of $\tilde{A}'$. Hence,

$$d_\tau^2 \psi_\chi^\tau + \tilde{\alpha}_c (\psi_\chi^{\tau+1} - \psi_\chi^{\tau-1}) - \tilde{\nu}_c^2 d_\chi^2 \psi_\chi^\tau = \text{Re}(\tilde{A}') \delta_{\chi,0} \Theta(\tau) e^{i\omega\tau\Delta t} \quad (5.68)$$

is an excellent model for most calculations.

When the source is turned on slowly, just as with the undamped case, the accuracy improves. S-FDTD and NS-FDTD calculations are given in Program MC5.1.

5.4 Time Reversal

In the simple wave equation given by Eq. (5.1), let $t \rightarrow t' = -t$. Then, defining ψ' by $\psi(x, t) = \psi'(x, t')$, we find that

$$\begin{aligned} \partial_t \psi(x, t) &= \partial_{t'} \psi'(x, t') \\ &= -\partial_{t'} \psi'(x, t'), \end{aligned} \quad (5.69)$$

$$\partial_t^2 \psi(x, t) = \partial_{t'}^2 \psi'(x, t'). \quad (5.70)$$

Since $\partial_x^2 \psi' = \partial_x^2 \psi$, the wave equation does not change its form under the operation of time reversal.

This has the practical consequence that we can run an FDTD calculation backwards. In the FDTD algorithm given by Eq. (5.3), at step 0 we input $\psi(x, 0)$ and $\psi(x, \Delta t)$, which we define as the state

$$\Psi^0 = \begin{bmatrix} \psi(x, 0) \\ \psi(x, \Delta t) \end{bmatrix}. \quad (5.71)$$

Iterating Eq. (5.3) to $t = (\tau + 1)\Delta t$, we obtain the state

$$\Psi^\tau = \begin{bmatrix} \psi(x, \tau\Delta t) \\ \psi(x, [\tau+1]\Delta t) \end{bmatrix}. \quad (5.72)$$

To effect time reversal, we simply replace Ψ^τ by

$$\Psi^\tau = \begin{bmatrix} \psi(x, [\tau+1]\Delta t) \\ \psi(x, \tau\Delta t) \end{bmatrix}; \quad (5.73)$$

in other words, we interchange the roles of $\psi[x, (\tau + 1)\Delta t]$ and $\psi(x, \tau\Delta t)\Delta t$ in the algorithm. Program MC5.2 is a simple demonstration of FDTD time reversal.

Time-reversed FDTD has been used in a variety of applications;^{3,4} the methodology has been extended to nonstandard FDTD,⁵ and various applications have been developed.⁶

Finally, it must be noted [see Eq. (5.69)] that an equation with a first derivative with respect to time is not invariant under time reversal. Thus, the absorbing wave equation as well as an absorbing computational boundary (see Chapter 6) are not time-reversal invariant.

Important Points of Chapter 5

- Standard (S) and nonstandard (NS) FDTD methodology for the wave equation and its variants are introduced.
- There is an exact NS-FDTD algorithm for the homogenous wave equation and its variants, and a nearly exact algorithm for the inhomogeneous wave equation.
- The NS amplitude of a source in free space is derived.
- To avoid large errors, sources must be turned on slowly in FDTD calculations.
- The stability condition for FDTD implies a speed limit on the grid as well as precursor waves.
- Time-reversed FDTD is discussed.

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Chapter 6

Program Development and Applications of FDTD Algorithms in One Dimension

In Chapter 5 we developed basic FDTD methodologies to solve the wave equation in its various forms, but to solve other problems of interest, we need to confront various ‘devils in the details.’

Topics:

- Terminating the computational boundary
- Extracting field intensity from FDTD calculations
- Simple object models on the grid
- Broadband NS-FDTD calculation
- Errors in the discrete Fourier transform methodology
- Scattered field calculation
- Discrete Green’s function methodology

6.1 The Computational Boundary

FDTD calculations are always carried out in a finite computational domain, such as

$$0 \leq x \leq N \Delta x, \quad (6.1)$$

where N is an integer. On the computational boundary ($x = 0$ and $x = N\Delta x$), $d_x^2\psi(x, t)$ is undefined because it requires values of $\psi(-\Delta x, t)$ and $\psi(N\Delta x + \Delta x, t)$, which lie outside of the computational domain and are therefore unknown. To iterate the FDTD algorithm, $d_x^2\psi$ must be defined on the boundary by some other method. There are three basic choices:

1. Reflecting computational boundary

Assume that ψ vanishes on and beyond the boundary so that

$$\psi(x, t) = 0 \quad \text{for } x \leq 0, \quad (6.2a)$$

$$\psi(x, t) = 0 \quad \text{for } x \geq N\Delta x. \quad (6.2b)$$

It is easy to demonstrate that this results in a reflecting boundary. A reflecting computational boundary is suitable for computing fields within a cavity with perfectly reflecting walls.

2. Periodic computational boundary

Assume ψ to be periodic on the boundary so that

$$\psi(-\Delta x, t) = \psi(N\Delta x, t), \quad (6.3a)$$

$$\psi(N\Delta x + \Delta x, t) = \psi(0, t). \quad (6.3b)$$

Thus,

$$d_x^2 \psi(0, t) = \psi(N\Delta x, t) + \psi(\Delta x, t) - 2\psi(0, t), \quad (6.4a)$$

$$d_x^2 \psi(N\Delta x, t) = \psi(0, t) + \psi(N\Delta x - \Delta x, t) - 2\psi(N\Delta x, t). \quad (6.4b)$$

The computational domain is now topologically equivalent to a circle. A wave that impinges on the left boundary emerges on the right, and vice versa. A periodic computational boundary is useful for modeling the propagation of a pulse in a long optical fiber, provided that $N\Delta x$ is much greater than the pulse width.

3. Absorbing computational boundary

Often neither a reflecting nor a periodic computational boundary is suitable. When light scatters from an object outdoors, it disappears for all practical purposes. In this case, we need what is called an absorbing (or transmitting) computational boundary, through which a wave appears to propagate and disappear as if the computational domain were infinite. In the computational electromagnetics literature, such a condition on the computational boundary is called an absorbing boundary condition (ABC).

6.1.1 One-way wave equations

The wave equation can be factored into

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = (\partial_t + v \partial_x)(\partial_t - v \partial_x) \psi(x, t) = 0, \quad (6.5)$$

and each factor yields what is called a one-way wave equation:

$$(\partial_t + v \partial_x) \psi(x, t) = 0, \quad (6.6a)$$

$$(\partial_t - v \partial_x) \psi(x, t) = 0. \quad (6.6b)$$

For an arbitrary function f it can be directly verified that the solutions of Eqs. (6.6a) and (6.6b) are $f(x - vt)$ and $f(x + vt)$, respectively. Since $\psi = f(x \mp vt)$ propagates in the $\pm x$ direction, Eq. (6.6a) is called the forward-wave equation and Eq. (6.6b) the backward-wave equation.

6.1.2 Finite difference models of the one-way wave equations

To implement an ABC in FDTD we need to construct finite difference models of the one-way wave equations on the boundaries at $b = 0$ and $b = N\Delta x$. Since we need to determine $\psi(b, t + \Delta t)$, we model ∂_t with a forward FD expression (see Section 1.1):

$$\begin{aligned}\Delta t \partial_t \psi(b, t) &\cong d_t^f \psi(b, t) \\ &= \psi(b, t + \Delta t) - \psi(b, t).\end{aligned}\quad (6.7)$$

To model the forward-wave equation using only points inside the computational domain, we model $\partial_x \psi(N\Delta x, t)$ in Eq. (6.6a) using a backward FD expression as

$$\begin{aligned}\Delta x \partial_x \psi(N\Delta x, t) &\cong d_x^b \psi(N\Delta x, t), \\ &= \psi(N\Delta x, t) - \psi(N\Delta x - \Delta x, t).\end{aligned}\quad (6.8)$$

Similarly, to model the backward-wave equation, we model ∂_x in Eq. (6.6b) using a forward FD expression:

$$\begin{aligned}\Delta x \partial_x \psi(0, t) &\cong d_x^f \psi(0, t), \\ &= \psi(\Delta x, t) - \psi(0, t).\end{aligned}\quad (6.9)$$

Thus, the forward- and backward-wave equation FD models and their corresponding FDTD algorithms are, respectively,

$$\begin{aligned}\left(d_t^f + \frac{v\Delta t}{\Delta x} d_x^b\right) \psi(x, t) &= 0 \quad \Rightarrow \\ \psi(x, t + \Delta t) &= \psi(x, t) + \frac{v\Delta t}{\Delta x} [\psi(x - \Delta x, t) - \psi(x, t)],\end{aligned}\quad (6.10a)$$

and

$$\begin{aligned}\left(d_t^f - \frac{v\Delta t}{\Delta x} d_x^f\right) \psi(x, t) &= 0 \quad \Rightarrow \\ \psi(x, t + \Delta t) &= \psi(x, t) + \frac{v\Delta t}{\Delta x} [\psi(x + \Delta x, t) - \psi(x, t)].\end{aligned}\quad (6.10b)$$

Using the methods of Appendix 7.1, it can be shown that the stability condition for the FDTD algorithms of Eq. (6.10) is

$$\frac{\nu\Delta t}{\Delta x} \leq 1. \quad (6.11)$$

In the special case where $\nu\Delta t/\Delta x = 1$, the above FD models and their corresponding FDTD algorithms are exact; thus,

$$(d_t^f + d_x^b)f(x - \nu t) = 0, \quad (6.12a)$$

$$(d_t^f - d_x^f)f(x + \nu t) = 0, \quad (6.12b)$$

for arbitrary f , and an exact ABC is

$$\psi(0, t + \Delta t) = \psi(\Delta x, t), \quad (6.13a)$$

$$\psi(N\Delta x, t + \Delta t) = \psi(N\Delta x - \Delta x, t). \quad (6.13b)$$

This ABC is useful in a variety of problems, where it is possible to set $\nu\Delta t/\Delta x = 1$ on the computational boundary, for example, a layered structure of refractive index > 1 immersed in vacuum.

Now evaluating Eq. (6.10a) with respect to a forward monochromatic wave $e^{i(kx - \omega t)}$, with $\omega = \nu k$ for $0 < \nu\Delta t/\Delta x < 1$, we find that

$$\left(d_t^f + \frac{\nu\Delta t}{\Delta x}d_x^b\right)e^{i(kx - \omega t)} = \varepsilon e^{i(kx - \omega t)}, \quad (6.14)$$

and we find the model error to be

$$\begin{aligned} \varepsilon &= (e^{-i\omega\Delta t} - 1) + u(1 - e^{-ik\Delta x}) \\ &= \frac{1}{2}u(1 - u)(k\Delta x)^2 - \frac{i}{6}u(1 - u^2)(k\Delta x)^3 + \cdots, \end{aligned} \quad (6.15)$$

where $u = \omega\Delta t/k\Delta x$. A similar result holds for Eq. (6.10b). The model error could be made to vanish by setting $u = (1 - e^{-i\omega\Delta t})/(1 - e^{-ik\Delta x})$, but a NS-FD model using complex u in place of $\nu\Delta t/\Delta x$ would not yield a useful ABC for real-valued waves. A better way is introduced below.

6.1.3 Central finite difference model of the one-way wave equations

The error in Eq. (6.15) is proportional to $(k\Delta x)^2$ because the forward and backward FD approximations are only first-order accurate. The model error can be reduced by employing central FD approximations, which are second-order accurate.

Note 6.1

Just as the errors of second-order FD approximations to derivatives partially cancel in the full wave equation to yield fourth-order accuracy, the errors of the first-order FD approximations in the one-way wave equations partially cancel to yield second-order accuracy.

The models [Eq. (6.10)] of the one-way wave equations are implemented on the boundaries ($x = 0$ and $x = N\Delta x$) at times $t = \tau\Delta t$ ($\tau = 0, 1, 2, \dots$), using forward- and backward-FD expressions. Since central FDs are generally more accurate than forward- and backward-FD expressions, let us try to improve the accuracy by modeling the one-way wave equations on the midpoints, $x = \Delta x/2$ and $x = N\Delta x - \Delta x/2$, and at half-time steps $t = \tau\Delta t + \Delta t/2$ using central FD expressions.

Writing $\psi(\chi \Delta x, \tau \Delta t) = \psi_\chi^\tau$ ($\chi = \text{integer}$), we model

$$(\partial_t + v\partial_x)\psi(N\Delta x - \Delta x/2, t + \Delta t/2) = 0 \quad (6.16)$$

by

$$(d_t + u d_x)\psi(N\Delta x - \Delta x/2, t + \Delta t/2) = 0, \quad (6.17a)$$

or by the equations that follow.

Central FD model of the forward wave equation:

$$\psi_{N-1/2}^{\tau+1} - \psi_{N-1/2}^\tau + u(\psi_N^{\tau+1/2} - \psi_{N-1}^{\tau+1/2}) = 0. \quad (6.17b)$$

Using the approximations

$$\psi_{N-1/2}^\tau \cong \frac{\psi_{N-1}^\tau + \psi_N^\tau}{2}, \quad (6.18)$$

$$\psi_\chi^{\tau+1/2} \cong \frac{\psi_\chi^{\tau+1} + \psi_\chi^\tau}{2}, \quad (6.19)$$

we obtain

$$(\psi_N^{\tau+1} + \psi_{N-1}^{\tau+1}) - (\psi_N^\tau + \psi_{N-1}^\tau) + u[(\psi_N^{\tau+1/2} + \psi_{N-1}^{\tau+1/2}) - (\psi_N^{\tau+1/2} + \psi_{N-1}^{\tau+1/2})] = 0, \quad (6.20)$$

and solving for $\psi_N^{\tau+1}$, we find the ABC at $x = N\Delta x$ to be as follows:

Standard ABC on the right:

$$\psi_N^{\tau+1} = \psi_{N-1}^{\tau} + \left(\frac{1-u}{1+u} \right) (\psi_N^{\tau} - \psi_{N-1}^{\tau+1}). \quad (6.21)$$

$\psi_{N-1}^{\tau+1}$ is computed using the FDTD algorithm for the (two-way) wave equation, while ψ_N^{τ} is known from the previous step.

Similarly, we model

$$(\partial_t - \nu \partial_x) \psi(\Delta x/2, \tau + \Delta t/2) = 0 \quad (6.22)$$

by the following:

Backward wave equation model:

$$(\psi_0^{\tau+1} + \psi_1^{\tau+1}) - (\psi_0^{\tau} + \psi_1^{\tau}) - u \left[(\psi_1^{\tau} + \psi_1^{\tau+1}) - (\psi_0^{\tau} + \psi_0^{\tau+1}) \right] = 0 \quad (6.23)$$

to obtain the ABC at $x = 0$.

Standard ABC on the left:

$$\psi_0^{\tau+1} = \psi_1^{\tau} - \left(\frac{1-u}{1+u} \right) (\psi_1^{\tau+1} - \psi_0^{\tau}). \quad (6.24)$$

Assuming a vanishing initial ($t = 0$) field on the boundary, we set $\psi_0^0 = \psi_N^0 = 0$ and can subsequently compute $\psi_N^{\tau>0}$ and $\psi_0^{\tau>0}$. For the case where $u = 0$, both Eqs. (6.21) and (6.24) reduce to the perfect ABC of Eq. (6.13).

Evaluating the model error of Eq. (6.20), we find that

$$\begin{aligned} \varepsilon &= 4i[-\sin(\omega \Delta t/2) \cos(k \Delta x/2) + u \cos(\omega \Delta t/2) \sin(k \Delta x/2)] \\ &= -\frac{i}{6}u(1-u^2)(k\Delta x)^3 - \frac{i}{240}u(1-u^4)(k\Delta x)^5 - \dots \end{aligned} \quad (6.25)$$

with a similar result at the $x = N\Delta x$ boundary. We have thus achieved third-order accuracy with this model.

6.1.4 Nonstandard finite difference model of the one-way wave equations

Now the model error can be made to vanish by setting $u = \tilde{v}_1$, where

$$\tilde{v}_1 = \frac{\tan(\omega \Delta t/2)}{\tan(k \Delta x/2)}. \quad (6.26)$$

Thus, an exact NS-ABC with respect to monochromatic waves for all values of $0 < \nu \Delta t / \Delta x \leq 1$ is as follows:

Exact nonstandard ABC:

$$\psi_N^{\tau+1} = \psi_{N-1}^{\tau} + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) (\psi_N^{\tau} - \psi_{N-1}^{\tau+1}), \quad (6.27a)$$

$$\psi_0^{\tau+1} = \psi_1^{\tau} - \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) (\psi_1^{\tau} - \psi_0^{\tau+1}). \quad (6.27b)$$

In the case where $v\Delta t/\Delta x = 1 \Rightarrow \tilde{v}_1 = 1$, Eq. (6.27) reduces to the perfect ABC of Eq. (6.13).

Different computational boundary conditions, including the ABC of Eq. (6.27), are implemented in Program MC.6.1.

6.2 Extracting Field Intensity from a Calculation

Physical measurements of light or sound usually yield the intensity. Intensity is the power per unit area transmitted by a wave. For a plane wave of amplitude $A = |\psi|$ (ψ may be complex), intensity is proportional to A^2 (see Appendix 4.1). We now show how to economically extract $|\psi(x, t)|^2$ from an FDTD computation of $\psi(x, t)$.

For a harmonic field of angular frequency ω , the computed time dependence at a fixed position can be modeled by

$$f(t) = A \sin(\omega t + \phi) + b + N(t), \quad (6.28)$$

where ϕ is the phase, b is some constant offset, and N is random noise. The noise can arise from precursor waves, which do not necessarily have a well-defined frequency, or from computational error.

For the zero-noise case ($N = 0$), it easy to show that

$$A^2 = \left[\frac{f'(t)}{\omega} \right]^2 + \left[\frac{f''(t)}{\omega^2} \right]^2. \quad (6.29)$$

Using nonstandard finite difference expressions,

$$f'(t) = \frac{f(t + \Delta t) - f(t - \Delta t)}{2 \sin(\omega \Delta t)/\omega}, \quad (6.30a)$$

and

$$f''(t) = \frac{f(t + \Delta t) + f(t - \Delta t) - 2f(t)}{-4 \sin^2(\omega \Delta t/2)/\omega^2}, \quad (6.30b)$$

exactly. Thus,

$$A^2 = \frac{[f(t + \Delta t) - f(t - \Delta t)]^2}{4 \sin^2(\omega \Delta t)} + \frac{[f(t + \Delta t) + f(t - \Delta t) - 2f(t)]^2}{16 \sin^4(\omega \Delta t/2)}. \quad (6.31)$$

Writing $\psi(x, \tau \Delta t) = \psi_x^\tau$, the amplitude of ψ in a FDTD calculation is thus

$$A^2 = \frac{(\psi_x^{\tau+1} - \psi_x^{\tau-1})^2}{4 \sin^2(\omega \Delta t)} + \frac{(\psi_x^{\tau+1} + \psi_x^{\tau-1} - 2\psi_x^\tau)^2}{16 \sin^4(\omega \Delta t/2)}. \quad (6.32)$$

If the noise amplitude is small compared to $|\psi_x^{\tau+1} - \psi_x^\tau|$, then formula Eq. (6.32) gives a very good result, but the longer the wavelength (and hence the longer the wave period) the smaller $|\psi_x^{\tau+1} - \psi_x^\tau|$ is relative to the noise. To ameliorate this problem, we use a larger sampling interval. Putting $\Delta t \rightarrow q\Delta t$, where q is a positive integer, Eq. (6.32) becomes

$$A^2 = \frac{(\psi_x^{\tau+q} - \psi_x^{\tau-q})^2}{4 \sin^2(\omega q \Delta t)} + \frac{(\psi_x^{\tau+q} + \psi_x^{\tau-q} - 2\psi_x^\tau)^2}{16 \sin^4(\omega q \Delta t/2)}. \quad (6.33)$$

To maximize $|\psi_x^{\tau+q} - \psi_x^\tau|$ without violating the Nyquist sampling criterion, we choose

$$q = \text{gilt}(T/8\Delta t), \quad (6.34)$$

where “gilt” denotes “the greatest integer less than” [for example, $\text{gilt}(8.9) = 8$].

This nonstandard intensity calculation and its performance are implemented in Program MC6.2.

6.3 Zero-Order Object Models on the Grid

As an example, let us set up an FDTD calculation of transmission through a layer of width w immersed in a medium, relative to which its index of refraction is n_s (Fig. 6.1). On the computational domain $0 \leq x \leq a$, we define the layer by

$$\begin{aligned} n &= 1 \text{ for } 0 \leq x \leq b \text{ and } b + w \leq x \leq a, \\ n &= n_s \text{ for } b \leq x \leq b + w. \end{aligned} \quad (6.35)$$

Discretizing time by $t = \tau \Delta t$, where $\tau = 0, 1, 2, \dots$, let $x = \chi \Delta x$, where $\chi = 0, 1, 2, \dots, N$, and $N\Delta x = a$.

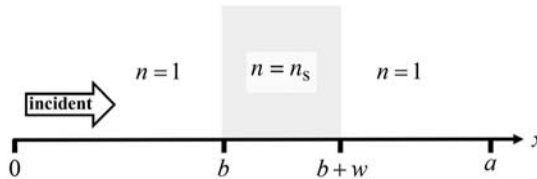


Figure 6.1 Setup to compute transmission through a layer of width w .

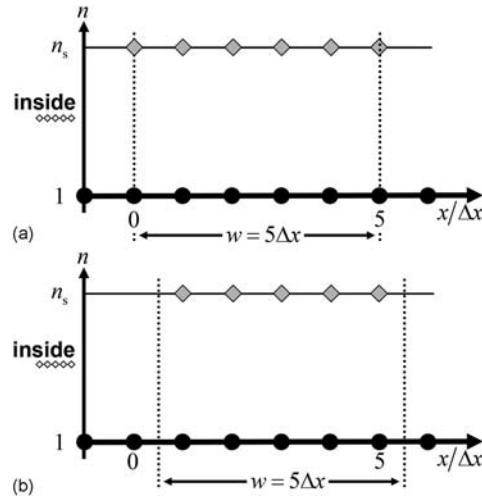


Figure 6.2 Representation of a layer on the numerical grid with layer edges on (a) the grid points and (b) between the grid points.

We now encounter a devil in the details: how to represent the layer on the numerical grid. For simplicity, let $w/\Delta x$ be an integer. The two most obvious choices are depicted in Fig. 6.2. In Fig. 6.2(a), the layer edges lie on the grid points, and in Fig. 6.2(b) the layer edges lie between the grid points.

Integrating $n(x) - 1$ over the computational domain, we obtain

$$\int_0^a [n(x) - 1] dx = (n_s - 1)w. \quad (6.36)$$

Summing over the grid points in representation Fig. 6.2(a) gives

$$\Delta x \sum_{\chi=0}^N [n(\chi\Delta x) - 1] = (n_s - 1)(w + \Delta x), \quad (6.37a)$$

and representation Fig. 6.2(b) gives

$$\Delta x \sum_{\chi=0}^N [n(\chi\Delta x) - 1] = (n_s - 1)w. \quad (6.37b)$$

Since the summation in Eq. (6.37b) is identical to the integral in Eq. (6.36), we conclude that the representation in Fig. 6.2(b) is better than that in Fig. 6.2(a). This can be confirmed by comparing the transmission or reflection spectrum of the layer computed analytically with an NS-FDTD calculation.

To compute the transmission of just one layer, it is always possible to choose $w/\Delta x$ to be an integer (by adjusting the value of Δx), but when there are many layers of different widths and spacings, this may not be possible. The case when $w/\Delta x$ is not an integer is discussed in Section 7.6. When $w/\Delta x$ is a noninteger, the model error is larger than when it is an integer.

6.4 Setting up an FDTD Calculation

The wave equation to be solved is

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \partial_x^2 \right) \psi_s(x, t) = \Theta(t) s(x, t), \quad (6.38)$$

where $n = n_s$ inside the layer and $n = 1$ outside. With reference to Fig. 6.1, we can set (source) $s = 0$ and specify the incident field by $\psi(x, 0)$ and $\psi(x, \Delta t)$, as shown in Fig. 6.3. The initial fields must be chosen to vanish in front of the layer because we do not know the fields inside the layer and beyond it. As long as the initial fields satisfy the boundary conditions on the layer boundary (and null fields do), the iteration of the FDTD algorithm automatically incorporates the boundary conditions on the layer interfaces. Alternatively, the incident field can be generated by a source, in which case, $\psi(x, 0) = \psi(x, \Delta t) = 0$. For example, to compute the transmission coefficient of an infinite plane wave, the incident field can be generated by a harmonic source. After a sufficient number of iterations, the FDTD solution converges to the analytic solution (see Note 4.5), provided that it is a sufficiently accurate model of the wave equation.

Figure 6.3 also give a heuristic explanation of how errors arise in FDTD calculations. If $v\Delta t/\Delta x = 1$, then the $\psi(x, \Delta t)$ waveform has exactly the same shape as $\psi(x, 0)$, but if $0 < v\Delta t/\Delta x < 1$, then $\psi(x, \Delta t)$ is distorted because it is not commensurate with the spatial grid.

Since n_s is the refractive index of the layer relative to the ambient medium in which it is immersed, we can always take the refractive index of the ambient medium to be 1 (Fig. 6.4). The physical values of the two refractive indices do not matter; only their ratio is important. For example, a layer of refractive index 3 immersed in a medium of refractive index 2 is equivalent to a layer of refractive index 1.5 immersed in a medium of refractive index 1. Similarly, a layer of physical refractive index 2 immersed in a medium of refractive index 3 is equivalent to layer of refractive index 2/3 immersed in a medium of refractive index 1.

The FDTD algorithm becomes

$$\psi_\chi^{\tau+1} = -\psi_\chi^{\tau-1} + \left(2 + \frac{1}{n_\chi^2} \frac{v_0^2 \Delta t^2}{\Delta x^2} d_\chi^2 \right) \psi_\chi^\tau + \Theta_g(t) s|_\chi^t \quad (6.39)$$

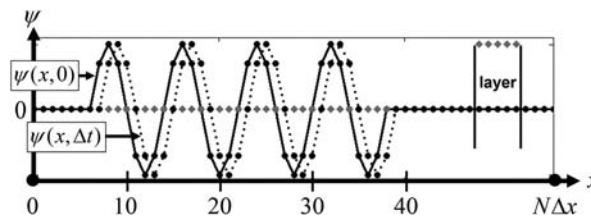


Figure 6.3 Pulse incident on a layer.

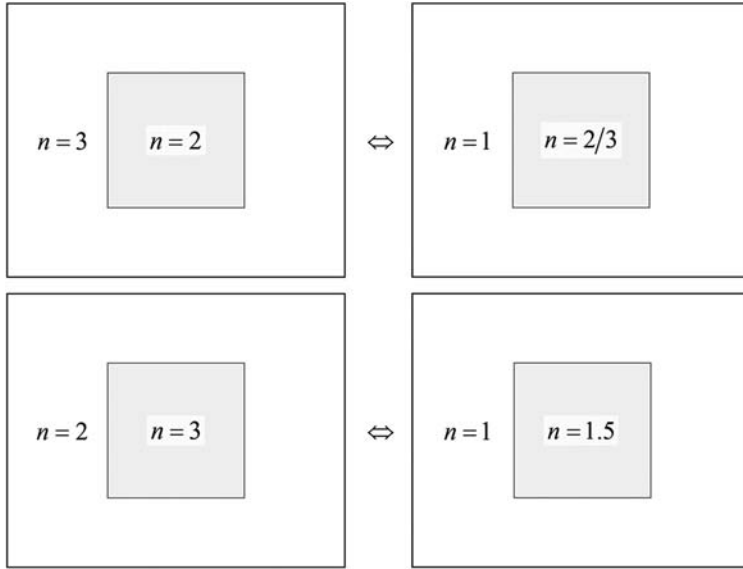


Figure 6.4 Equivalent models of an object immersed in an ambient medium.

for $1 \leq \chi \leq N-1$, where ν_0 is the propagation velocity in the ambient medium. The layer lies on the interval $b \leq x \leq b+w$. Using the representation of Fig. 6.2(b), we take $b = (\chi_b + \frac{1}{2})\Delta x$ and $b+w = (\chi_b + \frac{1}{2} + \Delta\chi)$, where χ_b and $\Delta\chi$ are integers. Thus, $n_\chi = 1$ for $0 \leq \chi \leq \beta$ and $\chi_b + \Delta\chi \leq \chi \leq N$, and $n_\chi = n_s$ for $\chi_b + \chi_b < \chi < \chi_b + \Delta\chi$.

6.4.1 Parameter choice

For wavelength λ and period T , the values of Δx are Δt are constrained by the Nyquist limits $\lambda/\Delta x > 2$ and $T/\Delta t > 2$, but to ensure reasonable accuracy it is advisable to take

$$\frac{\lambda}{\Delta x} \geq 4, \quad (6.40a)$$

$$\frac{T}{\Delta t} \geq 4. \quad (6.40b)$$

To model the layer on the grid, the larger $w/\Delta x$ the better, but

$$\frac{w}{\Delta x} \geq 1 \quad (6.41)$$

might be sufficient, depending on the problem. For propagation velocity $\nu = \lambda/T$, the stability condition $\nu\Delta t/\Delta x \leq 1$ must also be satisfied.

The absolute physical values and physical units of Δx and Δt do not matter. Only their ratios to the other physical quantities in the problem are important; thus, without loss of generality, we can set $\Delta x = \Delta t = 1$. From now on (unless otherwise specified), in all FDTD programs, we express length and time in units of Δx and Δt , respectively. Thus, $\lambda/\Delta x \rightarrow \lambda$, $T/\Delta t \rightarrow T$, $w\Delta x \rightarrow w$, and $\nu\Delta t \rightarrow \nu$. In the layer problem, $x = 0, 1, \dots, N$ and $t = 0, 1, \dots$. In the FDTD algorithm, the condition given by Eqs. (6.40) and (6.41) become

$$\lambda \geq 4, \quad (6.42a)$$

$$T \geq 4, \quad (6.42b)$$

$$w \geq 1, \quad (6.43)$$

and the stability condition becomes

$$\frac{\lambda}{T} \leq 1. \quad (6.44)$$

The FDTD algorithms for the layer problem can now be summarized. If $n_s > 1$ (high-refractive-index layer immersed in a low-refractive-index medium), we take $\nu_0 = 1$ so that the FDTD algorithm is exact (see Section 5.1.2) outside the layer, and the exact ABC given by Eq. (6.13) can be used. If $0 < n_s < 1$ (low-refractive-index layer immersed in a high-refractive-index medium), we take $\nu_0 = n_s < 1$ so that the FDTD algorithm is exact within the layer, but now we cannot use the exact ABC of Eq. (6.13).

Case 1: $n_s > 1$, on $1 \leq x \leq N - 1$

S-FDTD:

$$\psi_x^{t+1} = -\psi_x^{t-1} + \left(2 + \frac{1}{n_x^2} d_x^2\right) \psi_x^t, \quad (6.45)$$

where $n_x = n_s$ inside the layer, and $n_x = 1$ outside the layer.

NS-FDTD:

$$\psi_x^{t+1} = -\psi_x^{t-1} + \left(2 + \frac{1}{\tilde{n}_x^2} d_x^2\right) \psi_x^t, \quad (6.46)$$

where $n_x = n_s$ inside the layer, and $n_x = 1$ outside the layer. Recall from Section 5.1.3 that

$$\tilde{n} = \frac{\sin(n k_0 \Delta x / 2)}{\sin(k_0 \Delta x / 2)} \quad (6.47)$$

is the effective index of refraction on the grid for NS-FDTD.

In both S- and NS-FDTD, we use the perfect ABC given by Eq. (6.13) in the form

$$\psi_0^{t+1} = \psi_1^t, \quad (6.48a)$$

$$\psi_N^{t+1} = \psi_{N-1}^t. \quad (6.48b)$$

Case 2: $n_s < 1$, on $1 \leq x \leq N - 1$

S-FDTD:

$$\psi_x^{t+1} = -\psi_x^{t-1} + \left(2 + \frac{n_s^2}{n_x^2} d_x^2 \psi_x^t\right) + \Theta_g(t) s|_x^t, \quad (6.49)$$

where $n_x = n_s$ inside the layer, and $n_x = 1$ outside the layer. The update on the computational boundary using Eqs. (6.21) and (6.24) becomes

$$\psi_0^{t+1} = \psi_1^t - \left(\frac{1 - n_s}{1 + n_s}\right)(\psi_1^{t+1} - \psi_0^t), \quad (6.50a)$$

$$\psi_N^{t+1} = \psi_{N-1}^t + \left(\frac{1 - n_s}{1 + n_s}\right)(\psi_N^t - \psi_{N-1}^{t+1}). \quad (6.50b)$$

NS-FDTD:

$$\psi_x^{t+1} = -\psi_x^{t-1} + \left(2 + \frac{\tilde{n}_s^2}{\tilde{n}_x^2} d_x^2 \psi_x^t\right) + \Theta_g(t) \tilde{s}|_x^t, \quad (6.51)$$

where $n_x = n_s$ inside the layer, $n_x = 1$ outside the layer, and $\tilde{s}$ is the NS model of the source. The computational boundary is updated following Eq. (6.27) by

$$\psi_0^{t+1} = \psi_1^t - \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1}\right)(\psi_1^t - \psi_0^{t+1}), \quad (6.52a)$$

$$\psi_N^{t+1} = \psi_{N-1}^t + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1}\right)(\psi_N^t - \psi_{N-1}^{t+1}), \quad (6.52b)$$

where $\tilde{v}_1 = \tan(\omega_0/2)/\tan(k_0/2)$.

A pulse such as that shown in Fig. 6.3 contains a band of wavelengths. To obtain a high-accuracy solution with FDTD, the spatial discretization must be set such that Eq. (6.41a) holds for the shortest wavelength component we wish to consider.

6.5 The Scattered Field

If the incident field is an infinite plane wave (the case in most analytic calculations) and we wish to compute the reflected (scattered) field, it is convenient to compute it directly rather than extract it from a total field calculation.

Recall that the scattered-field wave equation is

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \partial_x^2\right) \psi_s(x, t) = \Theta(t) s_0(x, t), \quad (6.53)$$

where

$$\begin{aligned} s_0(x, t) &= -\left(\frac{n_s^2 - 1}{n_s^2}\right) \partial_t^2 \psi_0(x, t) & \text{for } x \in S \\ &= 0 & \text{for } x \notin S, \end{aligned} \quad (6.54)$$

where S is the set of points inside the scatterer. We now proceed to construct finite difference models for the scattered field.

6.5.1 Standard finite difference model

As we saw in Section 5.5.3, when a source is suddenly switched on in an FDTD calculation, transient fields are produced that can cause large errors, so we replace the step function in Eq. (6.53) with the Gaussian turn-on function Θ_g , defined in Eq. (5.56b). The S-FD model of the scattered field wave equation is thus

$$\left[d_t^2 - \frac{v_0^2 \Delta t^2}{n(x)^2 \Delta x^2} d_x^2\right] \psi_s(x, t) = \Delta t^2 \Theta_g(t) s_0(x, t). \quad (6.55)$$

Its corresponding S-FDTD algorithm

$$\psi_s(x, t + \Delta t) = -\psi_s(x, t - \Delta t) + \left[2 + \frac{v_0^2 \Delta t^2}{n(x)^2 \Delta x^2} d_x^2\right] \psi_s(x, t) + \Delta t^2 \Theta_g(t) s_0(x, t) \quad (6.56)$$

can be iterated from the initial fields

$$\psi_s(x, 0) = 0, \quad (6.57a)$$

$$\psi_s(x, -\Delta t) = 0. \quad (6.57b)$$

6.5.2 Nonstandard finite difference model

With respect to the incident field $\psi_0 = e^{i(k_0 x - \omega t)}$, an exact NS-FD model of the wave equation is

$$(d_t^2 - \tilde{v}_0^2 \partial_x^2) \psi_0(x, t) = 0, \quad (6.58)$$

where $\tilde{v}_0 = \sin(\omega \Delta t/2) / \sin(k_0 \Delta x/2)$. A nearly exact NS-FD model of the total field is

$$\left(d_t^2 - \frac{\tilde{\nu}_0^2}{\tilde{n}^2} d_x^2\right) \psi(x, t) = 0, \quad (6.59)$$

where $\tilde{n} = \sin(n k_0 \Delta x/2) / \sin(k_0 \Delta x/2)$ (see Section 5.1.3) is the effective index of refraction on the numerical grid. This model would be exact if there were no error at the scatterer boundary. Subtracting Eq. (6.58) from Eq. (6.59), we obtain

$$\left(d_t^2 - \frac{\tilde{\nu}_0^2}{\tilde{n}^2} d_x^2\right) \psi_s(x, t) = \Theta_g(t) \tilde{s}_0(x, t), \quad (6.60)$$

where

$$\begin{aligned} \tilde{s}_0(x, t) &= -\left(\frac{\tilde{n}_s^2 - 1}{\tilde{n}_s^2}\right) d_t^2 \psi_0(x, t) \\ &= 4 \sin^2(\omega \Delta t/2) \left(\frac{\tilde{n}_s^2 - 1}{\tilde{n}_s^2}\right) \psi_0(x, t) \quad \text{for } x \in S \\ &= 0 \quad \text{for } x \notin S. \end{aligned} \quad (6.61)$$

The corresponding NS-FDTD algorithm is

$$\begin{aligned} \psi_s(x, t + \Delta t) &= -\psi_s(x, t - \Delta t) + \left(2 + \frac{\tilde{\nu}_0^2}{\tilde{n}^2} d_x^2\right) \psi_s(x, t) \\ &\quad + \Theta_g(t) \tilde{s}_0(x, t), \end{aligned} \quad (6.62)$$

and its iteration starts with the initial fields of Eq. (6.57).

Comparing the source amplitudes of the S- and NS-FD models with respect to ψ_0 , we find that

$$\frac{\tilde{s}_0(x, t)}{\Delta t^2 s_0(x, t)} = \frac{4 \sin^2(\omega \Delta t/2) n_s^2}{\omega^2 \Delta t^2} \frac{(\tilde{n}_s^2 - 1)}{\tilde{n}_s^2} \frac{1}{(n_s^2 - 1)}. \quad (6.63)$$

If, for example, $n_s = 2$, $\nu_0 \Delta t/x = 1$, which implies that $k_0 \Delta x = \omega \Delta t$, and taking $\lambda_0/\Delta x = 8$, where $\lambda_0 = 2\pi/k_0$, we find that

$$\frac{\tilde{s}(x, t)}{\Delta t^2 s_0(x, t)} = 0.895; \quad (6.64)$$

thus, the source amplitudes in the S- and NS-FDTD algorithms can be quite different.

6.5.3 Setup of a scattered-field computation

With reference to the layer defined in Section 6.3, and following the methodology of Section 6.4, we now set up an FDTD calculation of the scattered field.

Taking the incident field to be $\psi_0(x, t) = \sin(k_0x - \omega t)$, the scattered-field wave Eq. (6.53) becomes

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \partial_x^2 \right) \psi_s(x, t) = \Theta(t) s_0(x, t), \quad (6.65)$$

where

$$s_0(x, t) = \omega^2 \left(\frac{n^2 - 1}{n^2} \right) \sin(k_0x - \omega t), \quad (6.66)$$

$n_x = n_s$ inside the layer, and $n_x = 1$ outside the layer. Taking $\Delta x = \Delta t = 1$, the S- and NS-FDTD algorithms for the scattered field can now be summarized.

Case 1: $n_s > 1$, on $1 \leq x \leq N - 1$

S-FDTD:

$$\psi_s|_x^{t+1} = -\psi_s|_x^{t-1} + \left(2 + \frac{1}{n_x^2} d_x^2 \right) \psi_s|_x^t + \Theta_g(t) s_0|_x^t \quad \text{for } 1 \leq x \leq N - 1, \quad (6.67)$$

where $n_x = n_s$ inside the layer, and $n_x = 1$ outside the layer.

NS-FDTD:

$$\psi_s|_x^{t+1} = -\psi_s|_x^{t-1} + \left(2 + \frac{1}{\tilde{n}_x^2} d_x^2 \right) \psi_s|_x^t + \Theta_g(t) \tilde{s}_0|_x^t \quad \text{for } 1 \leq x \leq N - 1, \quad (6.68)$$

where $\tilde{n}_x = \tilde{n}_s$ inside the layer, and $\tilde{n}_x = 1$ outside the layer.

In both the S- and NS-FDTD we use the perfect absorbing boundary condition given by Eq. (6.13) in the form

$$\psi_s|_0^{t+1} = \psi_s|_1^t, \quad (6.69a)$$

$$\psi_s|_N^{t+1} = \psi_s|_{N-1}^t. \quad (6.69b)$$

Case 2: $n_s < 1$, on $1 \leq x \leq N - 1$

S-FDTD:

$$\psi_s|_x^{t+1} = -\psi_s|_x^{t-1} + \left(2 + \frac{n_s^2}{n_x^2} d_x^2 \right) \psi_s|_x^t + \Theta_g(t) s_0|_x^t \quad \text{for } 1 \leq x \leq N - 1, \quad (6.70a)$$

$$\psi_s|_0^{t+1} = \psi_s|_1^t - \left(\frac{1 - n_s}{1 + n_s} \right) (\psi_s|_1^{t+1} - \psi_s|_0^t), \quad (6.70b)$$

$$\psi_s|_N^{t+1} = \psi_s|_{N-1}^t + \left(\frac{1 - n_s}{1 + n_s} \right) (\psi_s|_N^t - \psi_s|_{N-1}^{t+1}). \quad (6.70c)$$

NS-FDTD:

$$\psi_s|_x^{t+1} = -\psi_s|_x^{t-1} + \left(2 + \frac{\tilde{n}_s^2}{\tilde{n}_x^2} d_x^2 \right) \psi_s|_x^t + \Theta_g(t) \tilde{s}_0|_x^t \text{ for } 1 \leq x \leq N-1, \quad (6.71a)$$

$$\psi_s|_0^{t+1} = \psi_s|_1^t - \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) (\psi_s|_1^{t+1} - \psi_s|_0^t), \quad (6.71b)$$

$$\psi_s|_N^{t+1} = \psi_s|_{N-1}^t + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) (\psi_s|_N^t - \psi_s|_{N-1}^{t+1}), \quad (6.71c)$$

where the NS source is

$$\tilde{s}_0(x, t) = 4 \sin^2(\omega/2) \left(\frac{\tilde{n}^2 - 1}{\tilde{n}^2} \right) \sin(k_0 x - \omega t). \quad (6.72)$$

We take the initial fields to $\psi_s|_x^{-1} = \psi_s|_x^0 = 0$. In the program implementation, it is advantageous to separate the spatial and time dependence of the source using $\sin(k_0 x - \omega t) = \sin(k_0 x) \cos(\omega t) - \cos(k_0 x) \sin(\omega t)$.

6.5.4 Transmission/reflection spectrum of a layer

The reflected and transmitted intensity spectrum of an object is of great physical interest. Now we encounter another ‘devil in the details.’ The physically important quantity is w/λ , where λ is the incident wavelength. To compute the spectrum, we thus have two choices: (1) fix w and vary λ , or (2) fix λ and vary w . Unless $w/\Delta x$ is large, choice 1 is best because of the errors that arise when $w/\Delta x$ is not an integer.

Neglecting dispersive effects, the spectrum of a layer of width $w = 2\Delta x$ on the wavelength range $8 \leq \lambda/\Delta x \leq 16$ is equivalent to that of a layer of width $w = 4\Delta x$ on the wavelength range $16 \leq \lambda/\Delta x \leq 32$. This second FDTD calculation is more accurate because the larger the $\lambda/\Delta x$ and $w/\Delta x$ the lower the error.

A common method to compute a spectrum is to propagate an input pulse into the object of interest. The transmission/reflection spectrum can then be found by comparing the Fourier amplitudes of the incident pulse with those of the transmitted/reflected pulse. These amplitudes are found using the discrete Fourier transform (DFT), but there are some ‘devils in the details’ of which we must beware.

The ‘devil’ in the DFT

Performed naively, a DFT analysis can yield a spectrum that is wildly different from the true spectrum. The result can depend strongly on the number of time samples used, and accuracy may increase only slowly with sample size and also fluctuate with changes in sample size.

For example, let $\psi_i(t) = \sum_{m=0}^{32} \sin(\omega_m t)$ and $\psi_t(t) = \sum_{m=0}^{32} A_m \sin(\omega_m t)$ be “incident” and “transmitted” signals, respectively, where $\omega_m = \omega_0 + (m/32)\Delta\omega$, $\Delta\omega = 2\pi/11 - 2\pi/31$, $\omega_0 = 2\pi/31$, and A_m are the transmitted amplitudes. Taking $t = 0, 1, 2, \dots, N$, we digitize the signals and then extract the incident and transmitted spectra using DFTs. Let $\tilde{\psi}_i = \text{DFT}[\psi_i]$, and $\tilde{\psi}_t^{(0)} = \text{DFT}[\psi_t]$ (DFTs of the incident and transmitted fields, respectively). We compute the transmitted spectrum by normalizing it with respect to the incident spectrum to obtain $|\tilde{\psi}_{t,j}| = |\tilde{\psi}_{t,j}^{(0)}|/|\tilde{\psi}_{i,j}|$. The discrete Fourier frequencies are $\omega'_j = 2\pi j/N$, where $j = 0, 1, \dots, N'$, and $N' = N/2$ or $(N+1)/2$ for even N and odd N , respectively. The values of ω'_j are, in general, different from those of the ω_m given above. In other words, the DFT frequencies are not the same as the source frequencies.

In the upper panel of Fig. 6.5, the (true) incident spectrum of ψ_i (black dots) is compared with the incident spectrum found using DFT analysis $|\tilde{\psi}_i|$ (blue dots) for $N = 100$ and $N = 1000$. Notice that the DFT frequencies are not the same as the input frequencies. In the lower panel, we compare the (true) transmitted spectrum (black dots) with the transmitted DFT spectrum $|\tilde{\psi}_t|$ (blue dots). As we can see, the DFT spectrum is quite different from the true spectrum.

This phenomenon can be understood by examining $\psi_i(t)$. As we can see in Fig. 6.6, ψ_i is a sequence of pulses, but on $0 \leq t \leq 100$ the sampled signal contains only one-half a pulse, while on $0 \leq t \leq 1000$ it contains one and one-half.

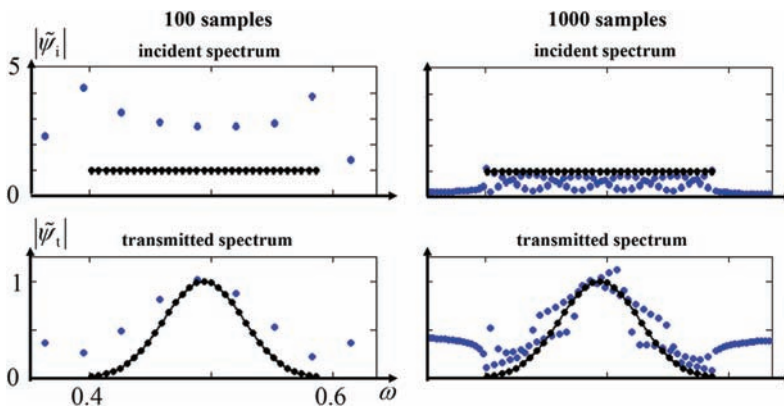


Figure 6.5 Discrete Fourier amplitude spectrum (blue dots) versus the true spectrum (black dots) on the angular frequency range $2\pi/31 \leq \omega \leq 2\pi/11$, $\Delta t = 1$. The DFT frequencies outside this range are numerical artifacts.

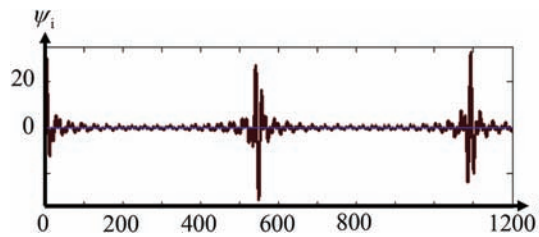


Figure 6.6 Incident signal ψ_i in the time domain.

Note 6.2

The pulses are not identical because the sampled signal is not strictly periodic. This because the true signal contains nonrational number periods that are incommensurate with the discrete time grid.

Let us now window the signal by taking a range that contains one entire pulse, such as $400 \leq t \leq 700$ (any “reasonable” range will do). Following the same procedure as before, we find the incident and transmitted spectra, shown in Fig. 6.7. This time the DFT analysis gives an excellent result.

The lesson is that one should examine the time-domain nature of the signal to be analyzed. In actuality, the DFT spectra of Fig. 6.5 are not wrong. They are the spectra of ψ_i and ψ_t on $0 \leq t \leq N$, but these samples are not a good model of the idealized signal that we want to investigate.

NS-FDTD spectrum calculation

We use a continuous-wave multifrequency source to generate the incident field. Let a wave containing angular frequencies ω_i ($i = 0, 1, \dots, N$) impinge on a layer of refractive index n_s . It is advisable to use evenly spaced frequencies, which produce a sequence of pulses, such as that shown in Fig. 6.6.

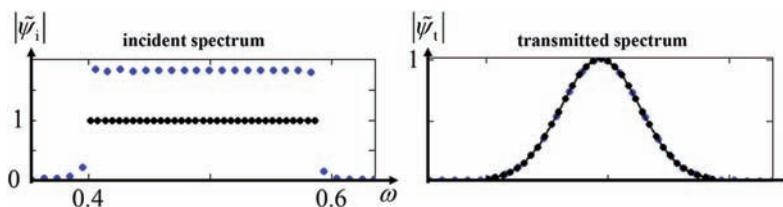


Figure 6.7 DFT analysis of the signal depicted in Fig. 6.6 sampled on $400 \leq t \leq 700$ (DFT spectrum (blue dots), true spectrum (black dots)). $|\tilde{\psi}_i|$ is relatively insensitive to the number of samples and the window position, as long as it contains the pulse.

In NS-FDTD, the wavenumber corresponding to ω_i is k_i , given by

$$\tilde{v} = \frac{\sin(\omega_i \Delta t/2)}{\sin(k_i \Delta x/2)}, \quad (6.73)$$

where $0 < \tilde{v} \leq 1$ is a constant with respect to frequency. Outside the layer, we can choose $\tilde{v} = \tilde{v}_O = 1$ (see Fig. 6.4); inside the layer, we set $\tilde{v} = \tilde{v}_L$. Because the relationship between ω_i and k_i is fixed by Eq. (6.73), $\sin(n_s k_i \Delta x/2) \neq \sin(\omega_i \Delta t/2)/\tilde{v}_L$ for all i . The effective index of refraction in the layer is

$$\tilde{n}_s(\tilde{v}_L)|_i = \frac{2}{k_i \Delta x} \arcsin \left[\frac{\sin(\omega_i \Delta t/2)}{\tilde{v}_L} \right]. \quad (6.74)$$

In general, $\tilde{n}_{s,i} \neq n_s$ and is different for each frequency. There are now two basic choices for $\tilde{v}_L$.

(1) Take $\tilde{v}_L = \tilde{v}_{L1}$, where

$$\tilde{v}_{L1} = \frac{\sin(\omega_N \Delta t/2)}{\sin(n_s k_N \Delta x/2)}, \quad (6.75)$$

and ω_N is the highest frequency. With this choice, the NS-FDTD error (within the layer) of the highest-frequency (shortest wavelength) component vanishes.

(2) Take $\tilde{v}_L = \tilde{v}_{L2}$, where

$$\tilde{v}_{L2} = \frac{\sin(\omega_0 \Delta t/2)}{\sin(n_s k_0 \Delta x/2)}, \quad (6.76)$$

and ω_0 is the lowest frequency. With this second choice, the NS-FDTD error (within the layer) of the lowest-frequency (longest wavelength) component vanishes. Of course, we could also choose some value of $\tilde{v}_L$ midway between $\tilde{v}_{L1}$ and $\tilde{v}_{L2}$ such that the effective refractive index equals n_s at some particular frequency. If the $\omega_i \Delta t$ values are sufficiently small, either choice will give a good result; otherwise, we can make two calculations and interpolate the results.

First compute spectrum 1 [$S^{(1)}$] with $\tilde{v}_L = \tilde{v}_{L1}$, and then spectrum 2 [$S^{(2)}$] with $\tilde{v}_L = \tilde{v}_{L2}$. From Eq. (6.74) the effective refractive indexes for $\tilde{v}_L = \tilde{v}_{L1}$ and $\tilde{v}_L = \tilde{v}_{L2}$ are, respectively,

$$\tilde{n}_s(\tilde{v}_{L1})|_i = \frac{2}{k_i \Delta x} \arcsin \left[\frac{\sin(\omega_i \Delta t/2)}{\sin(\omega_N \Delta t/2)} \sin(n_s k_N \Delta x/2) \right], \quad (6.77a)$$

$$\tilde{n}_s(\tilde{v}_{L2})|_i = \frac{2}{k_i \Delta x} \arcsin \left[\frac{\sin(\omega_i \Delta t/2)}{\sin(\omega_0 \Delta t/2)} \sin(n_s k_0 \Delta x/2) \right]. \quad (6.77b)$$

Obviously, $\tilde{n}_s(\tilde{v}_{L1})|_N = \tilde{n}_s(\tilde{v}_{L2})|_0 = n_s$. Plots of the $\tilde{n}_s(\tilde{v}_{L1})|_i$ and $\tilde{n}_s(\tilde{v}_{L2})|_i$ values are shown in Fig. 6.8 for the case $\tilde{v}_O = 1$ and $n_s = 2$. Finally, the

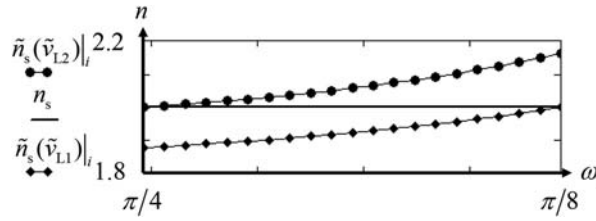


Figure 6.8 Effective refractive index for $\tilde{v}_L = \tilde{v}_{L1}$ and $\tilde{v}_L = \tilde{v}_{L2}$ as a function of angular frequency on the range $\pi/8 \leq \omega \Delta t \leq \pi/4$ for $n_s = 2$, $\Delta t = \Delta x = 1$.

frequency component i of the interpolated spectrum is computed by interpolating the two spectra to obtain

$$S_i = S_i^{(1)} + \left[\frac{n_s - \tilde{n}_s(\tilde{v}_{L1})|_i}{\tilde{n}_s(\tilde{v}_{L2})|_i - \tilde{n}_s(\tilde{v}_{L1})|_i} \right] [S_i^{(2)} - S_i^{(1)}]. \quad (6.78)$$

Program implementation and example calculation

Recall from Chapter 4, Eqs. (4.66) and (4.67), that a cosine point source generates a sine wave. From the discussion in Section 5.3.3, we saw that a cosine point source of angular frequency ω_i and amplitude

$$A_i = 4 \frac{\sin^2(\omega_i \Delta t/2)}{\sin(k_i \Delta x/2)} \quad (6.79)$$

generates a sine wave of unit amplitude in NS-FDTD, where $\sin(k_i \Delta x/2) = \sin(\omega_i \Delta t/2)/\tilde{v}$. Thus, a superposition of unit amplitude sine waves can be generated by the point source

$$s(x, t) = \delta_{x,p} \Theta_g(t) \sum_{i=0}^N A_i \cos(\omega_i t), \quad (6.80)$$

where Θ_g is the Gaussian turn-on function given by Eq. (5.56b), and $x = p$ is source position.

The first step is to set $n_s = 1$ and record the time dependence of the incident field at the sample point. A typical record is shown in Fig. 6.9 for an incident field containing 16 equally spaced angular frequencies on the band $2\pi/7 \leq \omega \Delta t \leq 2\pi/19$ with $\Delta x = \Delta t = 1$. The source is turned on slowly, and the sampling starts at $t = 256$. As noted above (the devil in the DFT), the signal is not exactly periodic.

To compute the transmission spectrum through a layer, the signal produced by the source is sampled on the opposite side of the layer. The setup together with a typical incident field ψ_i is shown in Fig. 6.10.

As discussed in the subsection called The ‘devil’ in the DFT, to compute the incident DFT spectrum I , a time sample that contains one or more pulses

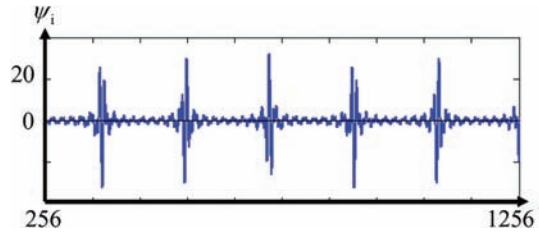


Figure 6.9 Incident field in the time domain used to compute the incident DFT spectrum.

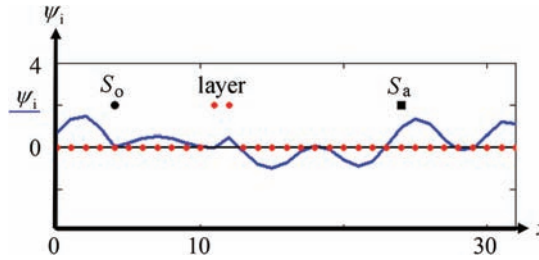


Figure 6.10 Incident field for a transmission spectrum calculation. The incident field ψ_i is generated at source point S_o and is sampled at S_a .

is used (blue dots in the graph labeled “incident spectrum” in Fig. 6.11). Ideally, the DFT frequencies and amplitudes would be identical to the input ones (black dots) on the range $\omega_0 \leq \omega \leq \omega_N$, but this not absolutely necessary.

Next we set n_s equal to the refractive index of the layer (in this example, $n_s = 2$, and layer width = $2\Delta x$). We run the program once with $\tilde{v}_L = \tilde{v}_{L1}$ to obtain spectrum $S^{(1)}$; then we run it again with $\tilde{v}_L = \tilde{v}_{L2}$ to obtain spectrum $S^{(2)}$.

Next we normalize $S^{(1)}$ and $S^{(2)}$ with respect to I ; thus, $S_i^{(1)} \rightarrow S_i^{(1)}/I_i$ and $S_i^{(2)} \rightarrow S_i^{(2)}/I_i$. In carrying out the normalization, frequency components with very small amplitudes should be filtered out of I lest they give rise to large errors.

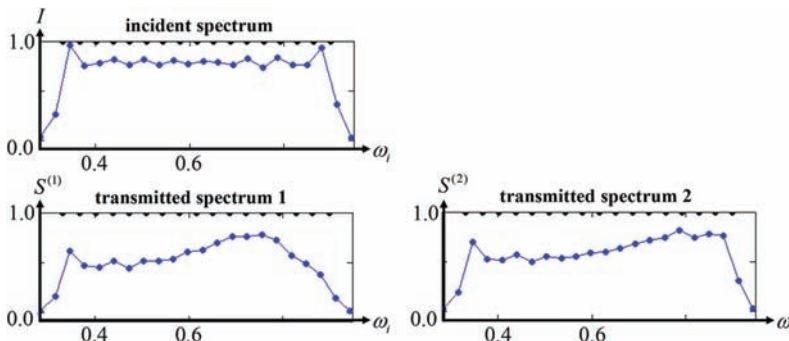


Figure 6.11 Incident intensity spectrum and two transmitted DFT intensity spectra from NS-FDTD calculations using 200 time samples for $256 \leq t < 456$, DFT amplitudes (blue dots) and amplitudes of incident angular frequencies (black dots).

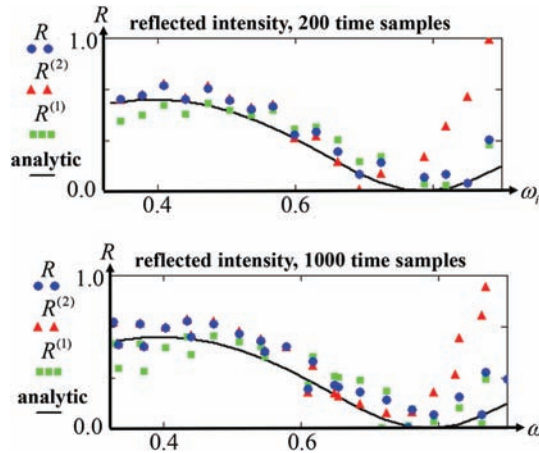


Figure 6.12 Reflected intensity spectrum from the data of Fig. 6.7. Computation using $S^{(1)}$ (green squares), using $S^{(2)}$ (red triangles), and using their interpolation, S (blue circles). The angular frequency range is $2\pi/7 \leq \omega\Delta t \leq 2\pi/19$ for $n_s = 2$; layer width = $2\Delta x$. Outside the angular frequency range, the error is large. $R^{(1)}$ is almost exact at the highest frequency, while $R^{(2)}$ is nearly exact at the lowest frequency.

Finally, using Eq. (6.78) we obtain the transmitted spectrum by interpolation. Subtracting each frequency component from unity gives the reflected intensity spectrum shown in Fig. 6.12, which is compared with the analytic spectrum obtained from layer theory (Appendix 4.3). Figure 6.12 shows the results for 200 and 1000 time samples starting at $t = 256$.

Returning to the ‘Devil in the DFT’ mentioned above, we see that increasing the number of time samples from 200 to 1000 yields little improvement in the overall accuracy. It is, however, possible to gain some improvement by cleverly choosing the time sample, as shown in Fig. 6.13, where 532 time samples starting at $t = 256$ were used to compute the incident DFT spectrum. Except where it vanishes, the DFT spectrum (blue dots) almost exactly matches the true incident spectrum (black dots on the black line). The zero amplitude components of I were filtered out to compute the transmission spectra.

Choosing a time sample for which the incident DFT spectrum most closely matches that of the incident field can improve the accuracy of the calculation to some extent, but ultimately it is necessary to use a finer grid to further increase the accuracy.

Doubling the layer width and halving each frequency (equivalent to doubling each incident wavelength), we repeat the calculations. As Fig. 6.14 shows, the NS-FDTD result almost exactly matches the analytic result. Now the interpolation discussed above is almost unnecessary. It would suffice to take $\tilde{v}_L = (\tilde{v}_{L1} + \tilde{v}_{L2})/2$ in a single computational run. As long as the incident DFT is calculated correctly, good accuracy can be expected.

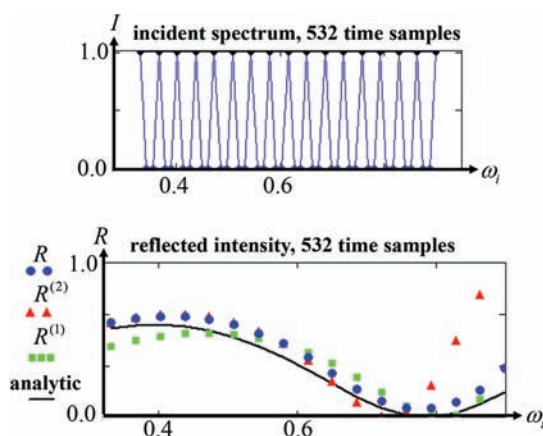


Figure 6.13 (Top) DFT intensity spectrum of the incident field and (bottom) the reflected intensity spectrum for a layer. Except for the number of time samples, all of the computation parameters are the same as in Fig. 6.12.

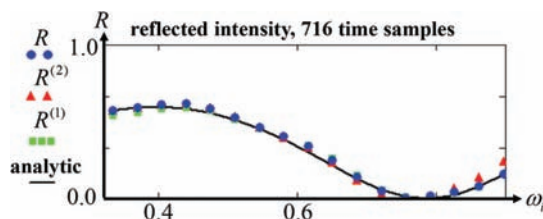


Figure 6.14 Reflected intensity spectrum from the data of Fig. 6.7. The slab width and each incident wavelength is doubled. Computation using $S^{(1)}$ (green squares), using $S^{(2)}$ (red triangles), and using their interpolation, S (blue circles). Frequency is scaled to that of Figs. 6.12 and 6.13. Time sampling starts at $t = 512$.

On a coarser grid, some improvement in accuracy can also be obtained by using narrower bandwidths at the expense of a larger number of computational runs.

Devil in the details

The spectrum calculation could also be done using a band of equally spaced wavelengths. In this case, the frequencies in Eq. (6.80) correspond to these wavelengths. However, instead of a sequence of pulses, such as that of Fig. 6.9, the time-domain signal would be much more complicated. The beginning and end of the optimum sample window is less obvious. In this case, the computed spectrum can be quite sensitive to the number of time samples used, and even on a fine grid, large errors can occur due to an unfortunate choice of the number of time samples and sampling window.

Program MC 6.3 uses NS-FDTD to compute the transmission spectrum of a layer.

6.6 Solution using Discrete Green's Functions

As we have seen in Section 4.3, an inhomogeneous wave equation can be solved analytically in terms of a Green's function—provided that it can be found. Even in relatively simple cases, however, such as the damped wave equation, it can be difficult to find the Green's function because it must satisfy the same initial and boundary conditions as the solution we seek. The practical use of Green's functions to solve problems analytically is thus rather limited.

However, Green's functions can be effectively used to solve finite difference models of the inhomogeneous (differential) wave equation and of Maxwell's equations. Although the Green's function g for a FD model of a differential equation is generically the same as the Green's function G for the differential equation itself, we call g the *discrete* Green's function (DGF) because it solves a difference equation at discrete space–time points, but is *not* a sampled version of G .

Let us now develop a DGF solution for a FD model of the inhomogeneous wave equation,

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = s(x, t), \quad (6.81)$$

where v may vary with position. The corresponding FD model is

$$(d_t^2 - u^2 d_x^2) \psi(x, t) = s_{\text{FD}}(x, t), \quad (6.82)$$

where u and s_{FD} are the FD models of $v\Delta t/\Delta x$ and s , respectively. Discretizing space–time by $x = \chi\Delta x$ and $t = \tau\Delta t$ (χ, τ integers), and writing $\psi(\chi\Delta x, \tau\Delta t) = \psi_\chi^\tau$, $s_{\text{FD}}(\chi\Delta x, \tau\Delta t) = s_{\text{FD}}|_\chi^\tau$, Eq. (6.82) becomes

$$(d_\tau^2 - u^2 d_\chi^2) \psi_\chi^\tau = s_{\text{FD}}|_\chi^\tau. \quad (6.83)$$

The most general DGF that solves this equation satisfies

$$(d_\tau^2 - u^2 d_\chi^2) g_{\chi, \chi'}^{\tau-\tau'} = \delta_{\chi, \chi'} \delta_{\tau, \tau'}. \quad (6.84)$$

Note 6.3

As we saw in Appendix 4.4, in general, $G = G(x, x'; t, t')$, although it is usually a function of $t - t'$ (but not necessarily of $x - x'$). Here we do not assume g to be a function of $\chi - \chi'$ (see Note A4.4.1).

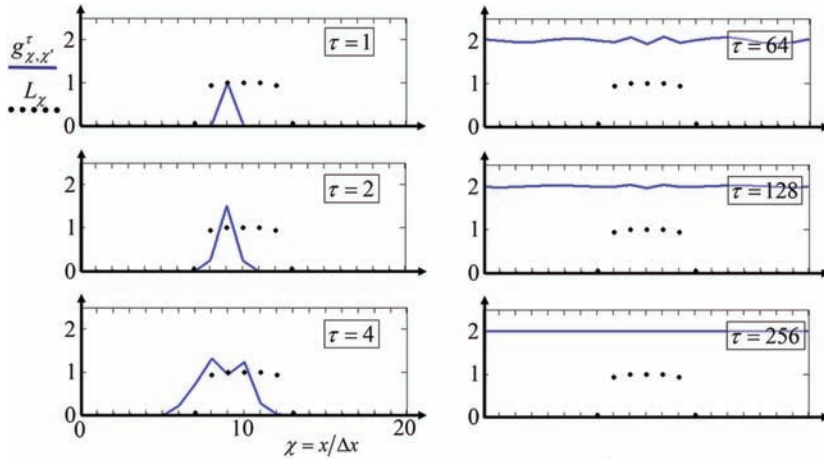


Figure 6.15 Time evolution of the discrete Green's function $g_{\chi, \chi'}^{\tau}$ for $\chi' = 9$ on the computational domain $0 \leq x/\Delta x \leq 20$ for scattering off a layer structure; $n_s = 1.5$.

Redefining τ , $\tau \rightarrow \tau - \tau'$, we take the initial conditions to be $\psi_{\chi, \chi'}^{-1} = \psi_{\chi, \chi'}^0 = 0$, and the DGF is given by the FDTD algorithm

$$g_{\chi, \chi'}^{\tau+1} = -g_{\chi, \chi'}^{\tau-1} + (2 + d_{\chi}^2)g_{\chi, \chi'}^{\tau} + \delta_{\chi, \chi'}\delta_{\tau, 0}. \quad (6.85)$$

Figure 6.15 depicts the time evolution of a DGF for a layered structure. The refractive index at $x = \chi\Delta x$ is $n_{\chi} = 1 + (L_{\chi} - 1)n_s$, where the “layer function” L_{χ} varies as shown, to give a spatially variable refractive index.

It is easy to show that the solution of the difference equation [Eq. (6.84)] is

$$\psi_{\chi}^{\tau} = \sum_{\tau'=-\infty}^{\infty} \sum_{\chi'=-\infty}^{\infty} g_{\chi, \chi'}^{\tau-\tau'} s_{\text{FD}}|_{\chi'}^{\tau'}. \quad (6.86)$$

To the extent that the FD model of the wave equation [Eq. (6.80)] is accurate, the solution of Eq. (6.81) is a sampled version of the solution of the wave equation.

The DGF for the simple case $u = \text{constant}$ everywhere is derived in Appendix 6.2. In this simple case there is an analytic solution, but in general we must find the DGF using Eq. (6.84).

Let us now apply the DGF methodology to the scattered-field calculation for the layer depicted in Fig. 6.15. Taking $\Delta x = \Delta t = 1$, we have $t = \tau$, $t' = \tau'$, $x = \chi$, and $x' = \chi'$, and we seek the DGF that solves

$$\left(d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} d_x^2\right) \psi_s(x, t) = s_{\text{FD}}(x, t). \quad (6.87)$$

Assuming all the source points of the scatterer to turn on at $t' = \tau'\Delta t = 0$, we seek the solution of

$$\left(d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} d_x^2\right) g|_{x,x'}^t = \delta_{x,x'} \delta_{t,0}. \quad (6.88)$$

Multiplying by $s_{\text{FD}}|_{x'}^t$ and summing over x' , we obtain

$$\left(d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} d_x^2\right) \sum_{x' \in S} g|_{x,x'}^t s_{\text{FD}}|_{x'}^t = s_{\text{FD}}|_x^t \delta_{t,0}. \quad (6.89)$$

Since the source of the scattered field vanishes outside the layer, the summation needs to be carried out only for the points within it. We call the solution of Eq. (6.89) the space-summed (SS) DGF, g_{SS} . The SS-DGF can be found using FDTD. Thus given g_{SS} , the solution of Eq. (6.87) becomes

$$\psi_\chi^r = \sum_{t'=0}^t g_{\text{SS}}|_x^{t-t'} s_{\text{FD}}|_x^{t'}. \quad (6.90)$$

The longer the wavelength the more accurate is S-FDTD. The advantage of NS-FDTD is seen at short wavelengths (high frequency); thus, in the DGF solution we take $\tilde{n}$ to be the effective refractive index for the highest frequency in the spectrum we wish to compute.

The DGF methodology is useful for computing the field due to different sources. The storage required to hold g_{SS} can be large, but the data can be compressed in places where the variation of g_{SS} is slow (either spatially or temporally) either by fitting it to an analytic function or by clever sampling.

DGFs have also been used to develop terminations of the FDTD computational domain.¹⁻⁴

Important Points of Chapter 6

- We show how to terminate the computational boundary using S- and NS-Mur absorbing boundary conditions.
- We show how to represent structures on the grid. Noninteger sizes (in terms of grid units) cause errors.
- The NS model of the source of the scattered field is different from the NS model of a source in free space.
- The analytical calculation of the scattered field and its FDTD computation are different, but the latter is a very good approximation to the former.
- We set up a multiple-frequency NS-FDTD calculation of a spectrum using the discrete Fourier transform
- Judiciously choosing the sample window and number of time samples in the discrete Fourier transform can improve accuracy, especially on a coarse grid. Care must be taken to filter out low-amplitude components of the incident DFT spectrum.

- We introduce the discrete Green's function for the wave equation, and discrete Green's function methods.

Appendix 6.1 Discrete Green's Function for the 1D Finite Difference Wave Equation

A6.1.1 Introduction

We derive the discrete Green's function (DGF) for a FD model of the inhomogeneous 1D wave equation

$$(\partial_t^2 - v^2 \partial_x^2) \psi(x, t) = s(x, t) \quad (\text{A6.1.1})$$

in free space with the initial conditions

$$\psi(x, t) = 0 \quad \text{for } t \leq 0, \quad (\text{A6.1.2a})$$

$$\partial_t \psi(x, t) = 0 \quad \text{for } t \leq 0. \quad (\text{A6.1.2b})$$

The source s , which turns on at $t = 0$, has the form $s(x, t) = \Theta(t)\sigma(x, t)$, where Θ is the step function.

We model the wave equation by the difference equation

$$(d_t^2 - u^2 d_x^2) \psi(x, t) = \Delta t^2 s(x, t). \quad (\text{A6.1.3})$$

In the S-FD model $u = v\Delta x/\Delta t$, and in the NS-FD model $u = \sin(\omega\Delta t/2)/\sin k\Delta x/2$.

We discretize space and time by $x = \chi\Delta x$ and $t = \tau\Delta t$, where χ and τ are integers; and we define $\psi(\chi\Delta x, \tau\Delta t) = \psi_\chi^\tau$ and $\Delta t^2 s(\chi\Delta x, \tau\Delta t) = s_\chi^\tau$. In this notation, Eq. (A6.1.3) becomes

$$(d_\tau^2 - u^2 d_\chi^2) \psi_\chi^\tau = s_\chi^\tau, \quad (\text{A6.1.4})$$

where $d_\tau^2 \psi_\chi^\tau = \psi_\chi^{\tau+1} + \psi_\chi^{\tau-1} - 2\psi_\chi^\tau$, and $d_\chi^2 \psi_\chi^\tau = \psi_{\chi+1}^\tau + \psi_{\chi-1}^\tau - 2\psi_\chi^\tau$.

This difference equation can be solved in terms of a discrete Green's function (DGF) g , which in unbounded free space satisfies

$$(d_\tau^2 - u^2 d_\chi^2) g_{\chi-\chi'}^{\tau-\tau'} = \delta_{\chi-\chi',0} \delta_{\tau-\tau',0}, \quad (\text{A6.1.5})$$

subject to the initial conditions

$$g_{\chi-\chi'}^{-1} = 0, \quad (\text{A6.1.6a})$$

$$g_{\chi-\chi'}^0 = 0, \quad (\text{A6.1.6b})$$

where δ is the Kronecker delta. It is easy to show that the solution of Eq. (A6.1.4) is given by

$$\psi_{\chi}^{\tau} = \Delta t^2 \sum_{\tau'=-\infty}^{\infty} \sum_{\chi'=-\infty}^{\infty} g_{\chi-\chi'}^{\tau-\tau'} s_{\chi'}^{\tau'}. \quad (\text{A6.1.7})$$

Note A6.1.1

The above is not the solution of the wave Eq. (A6.1.1), but rather the solution of its FD model, Eq. (A6.1.4). The closer this FD model is to the wave equation the closer ψ_{χ}^{τ} is to the wave equation solution.

A6.1.2 Derivation of the discrete Green's function

Without loss of generality, we can take $\chi' = 0$ and $\tau' = 0$ so that Eq. (A6.1.5) reduces to

$$(d_{\tau}^2 - u^2 d_{\chi}^2) g_{\chi}^{\tau} = \delta_{\chi,0} \delta_{\tau,0}. \quad (\text{A6.1.8})$$

Since the propagation is isotropic, $g_{-\chi}^{\tau} = g_{\chi}^{\tau}$. To ensure numerical stability in 1D FDTD, we must take

$$0 \leq u \leq 1, \quad (\text{A6.1.9})$$

which implies that

$$g_{\chi}^{\tau}|_{\chi \geq \tau} = 0. \quad (\text{A6.1.10})$$

This condition is just a form of causality. The initial conditions given by Eq. (A6.1.6) become

$$g_{\chi}^{-1} = 0, \quad (\text{A6.1.11a})$$

$$g_{\chi}^0 = 0, \quad (\text{A6.1.11b})$$

and g_{χ}^{τ} can then be evaluated directly using the FDTD algorithm. For example,

$$g_{\chi}^1 = -g_{\chi}^{-1} + 2g_{\chi}^0 + u^2 d_{\chi}^2 g_{\chi}^0 + \delta_{\chi,0} \delta_{0,0} = \delta_{\chi,0}. \quad (\text{A6.1.12})$$

This process can be repeated, and an expression for g_{χ}^{τ} is derived in Section A6.1.3, but this calculation is tedious and yields a very complicated expression.

There is a simpler approach. Let $k_n = 2\pi n/N$, where $n = 0, 1, \dots, N-1$, where $N \geq 1$ is an integer; and let $\sin(\omega_n/2) = u \sin(k_n/2)$. Using the identity

$d_\tau^2 e^{i\omega\tau}/e^{i\omega\tau} = -4\sin^2(\omega/2)$, a basis solution of Eq. (A6.1.8) for $\chi \neq 0$ and $\tau \neq 0$ is

$$\varphi_n|_\chi^\tau = [a_s \sin(k_n\chi) + a_c \cos(k_n\chi)] \times [b_s \sin(\omega_n\tau) + b_c \cos(\omega_n\tau)], \quad (\text{A6.1.13})$$

where a_s , a_c , b_s , and b_c are constants to be determined.

To satisfy the condition given by Eq. (A6.1.11b), we choose $b_c = 0$. We can replace the condition given by Eq. (A6.1.11a) with Eq. (A6.1.12) and satisfy it by taking $a_s = 0$, leaving the form $\varphi_n|_\chi^\tau = A_n \cos(k_n\chi) \sin(\omega_n\tau)$, where the constant A_n is to be determined. To φ_n we can add arbitrary functions of the form $f|_\chi^\tau = a\tau + b\chi + c$, where a , b , and c are constants (because $d_\tau^2 f|_\chi^\tau = d_\chi^2 f|_\chi^\tau = 0$). The solution of Eq. (A6.1.8) now has the form

$$g_\chi^\tau = a\tau + b\chi + c + \sum_{n=1}^{N-1} A_n \sin(\omega_n\tau) \cos(k_n\chi), \quad (\text{A6.1.14})$$

and we must now find A_n , a , b , and c such that Eqs. (A6.1.11b) and (A6.1.12) are satisfied for $0 \leq \chi < \tau$. For $0 \leq \chi \leq N-1$, $\delta_{\chi,0}$ can be expressed in the form

$$\delta_{\chi,0} = \frac{1}{N} + \frac{1}{N} \sum_{n=1}^{N-1} \cos(k_n\chi). \quad (\text{A6.1.15})$$

Note A6.1.2

For $\chi = 0$, the identity is obvious. For $\chi \neq 0$,

$$\sum_{n=0}^{N-1} e^{2\pi i n\chi/N} = (1 - e^{2\pi i\chi})/(1 - e^{2\pi i\chi/N}) = 0$$

because χ is an integer and $e^{2\pi i\chi/N} \neq 1$; thus, $\sum_{n=0}^{N-1} \cos(k_n\chi) = 0$ for $\chi \neq 0$. We have only the first term on the right of Eq. (A6.1.15) because there is no summation.

Choosing $A_n = 1/\sin(\omega_n)$, $a = 1/N$ and $b = 0$, we obtain

$$g_\chi^\tau = \frac{\tau}{N} + \frac{1}{N} \sum_{n=1}^{N-1} \frac{\sin(\omega_n\tau)}{\sin(\omega_n)} \cos(k_n\chi). \quad (\text{A6.1.16})$$

It can be directly verified that Eq. (A6.1.16) satisfies Eq. (A6.1.8) together with Eqs. (A6.1.11b) and (A6.1.12) for $0 \leq \chi \leq N-1$ and $0 \leq \tau \leq N-1$. Thus, to compute g_χ^τ for a fixed g_χ^τ , we set $N = \tau + 1$ in Eq. (A6.1.16). Using $\sin(\omega_n/2) = u \sin(k_n/2)$, g_χ^τ can be expressed directly in terms of u . It can be verified that Eq. (A6.1.16) is identical to the expression derived in Section A6.1.3.

A6.1.3 Derivation of the discrete Green's function using FDTD

We can now directly solve Eq. (A6.1.8). For notational brevity, we write $u^2 = U$, and represent g_χ^τ as a column vector g^τ , where the rows are ordered downwards from $\chi = 0, 1, 2, \dots$

The first few iterations yield

$$\begin{aligned}
 g^1 &= \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \quad g^2 = \begin{bmatrix} -2U + 2 \\ U \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \quad g^3 = \begin{bmatrix} 6U^2 - 8U + 3 \\ -4U^2 + 4U \\ U^2 \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix}, \\
 g^4 &= \begin{bmatrix} -20U^3 + 36U^2 - 20U + 4 \\ 15U^3 - 24U^2 + 10U \\ -6U^3 + 6U^2 \\ U^3 \\ 0 \\ 0 \\ \vdots \end{bmatrix}.
 \end{aligned} \tag{A6.1.17}$$

The dashed lines above the column matrices indicate symmetry about ($\chi = 0$) and that the matrices continue (upward) in the $-\chi$ direction.

Since $g_\chi^\tau = g_{-\chi}^\tau$, we need only to compute g_χ^τ . For the special case where $u = 1$, we can verify that

$$g(\chi, \tau) = \frac{1 - (-1)^{\tau-\chi}}{2} \Theta(\tau - |\chi|). \tag{A6.1.18}$$

For $u \neq 1$ and $\tau \geq 1$, g_χ^τ can be expressed in the general form

$$g_\chi^\tau = \sum_{n=|\chi|}^{\tau-1} \alpha_{\chi,n}^\tau U^n, \tag{A6.1.19}$$

where the coefficients $\alpha_{\chi,n}^\tau$ are to be determined. By inspection, we find that

$$g_{\tau-1}^{\tau-1} = U^{\tau-1}; \tag{A6.1.20}$$

hence, $\alpha_{\tau-1,\tau-1}^\tau = 1$, and the downward recursion relation is

$$\alpha_{\chi-1,n}^{\tau} = -\alpha_{\chi,n}^{\tau} \left(\frac{n+\chi}{n-\chi+1} \right). \quad (\text{A6.1.21})$$

The sum of the U^n coefficients satisfies

$$\sum_{n=|\chi|}^{\tau-1} \alpha_{\chi,n}^{\tau} = \frac{1 - (-1)^{\tau-\chi}}{2} \Theta(\tau - |\chi|), \quad (\text{A6.1.22})$$

and all of the $\alpha_{\chi,n}^{\tau}$ values can now be determined from Eqs. (A6.1.20) to (A6.1.22).

Actually, it is easier to first find g_0^{τ} , and then, using upward recursion, to determine g_{χ}^{τ} . Using downward recursion from $\alpha_{\tau-1,\tau-1}^{\tau} = 1$, we find that

$$\alpha_{0,\tau-1}^{\tau} = (-1)^{\tau-1} \frac{(2\tau-2)!}{[(\tau-1)!]^2}. \quad (\text{A6.1.23})$$

Now, using the fact that $d_{\tau}^{2n+1} \alpha_{0,n}^{\tau} = \alpha_{0,n}^{\tau}$ ($0 \leq n \leq \tau-1$), we can determine $\alpha_{0,n}^{\tau}$ to obtain

$$g_0^{\tau} = \sum_{n=0}^{\tau-1} \frac{(-1)^n}{(2n+1)} \frac{(\tau+n)!}{(\tau-n-1)!} \frac{u^{2n}}{(n!)^2}. \quad (\text{A6.1.24})$$

Upward recursion gives

$$\alpha_{\chi+1,n}^{\tau} = -\alpha_{\chi,n}^{\tau} \left(\frac{n-\chi}{n+\chi+1} \right). \quad (\text{A6.1.25})$$

The final expression is

$$g_{\chi}^{\tau}|_{\chi \geq 0} = \sum_{n=\chi}^{\tau-1} \frac{(-1)^{n+\chi}}{(2n+1)} \frac{(\tau+n)!}{(\tau-1-n)!} \frac{u^{2n}}{(n+\chi)!(n-\chi)!}. \quad (\text{A6.1.26})$$

A6.1.4 Interpretation and analysis

The discrete Green's function is the field due to impulse at $(x = 0, t = 0)$. For $u = \nu \Delta t / \Delta x = 1$, the leading edge of the wavefront is located at $|x| = \tau \Delta x$, but even when $u < 1$, the leading edge propagates as if $u = 1$ and is located at $|x| = \tau \Delta x$. On the other hand, the leading edge of the Green's function, $G(x, t) = \Theta(\nu t - |x|)/2\nu$, for the wave equation propagates with velocity ν . We compare $G(x, t)$ and $g(x, t)$ in Fig. A6.1.1.

While G vanishes for $|x| > \nu t$, g does not vanish until $|x| > t - \Delta t$, but it falls exponentially for $|x|/\Delta x > u(t/\Delta t)$. This implies that in the discretized wave equation, the main disturbance propagates with “velocity” $u < 1$, but a precursor signal propagates with a “velocity” of unity.

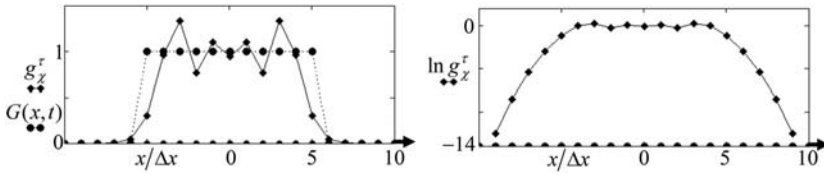


Figure A6.1.1 (left) $G(x, t)$ and $g(x, t)$ for $\nu = u = 1/2$ at $t = 10\Delta t$, $\Delta x = \Delta t = 1$. (right) $\log g$ plotted.

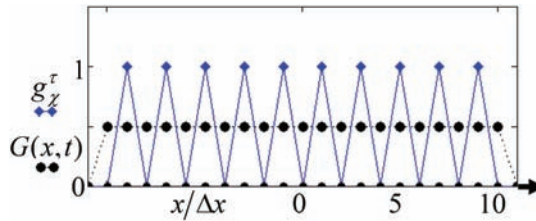


Figure A6.1.2 $G(x, t)$ (circles) and $g(x, t)$ (diamonds) for $\nu = u = 1$ at $t = 10\Delta t$, $\Delta x = \Delta t = 1$.

Although for $u = 1$, $(d_t^2 - u^2 d_x^2)\psi(x, t) = 0$ is an exact finite difference model of the homogeneous wave equation $(\partial_t^2 - v^2 \partial_x^2)\psi(x, t) = 0$, $(d_t^2 - u^2 d_x^2)\psi(x, t) = \Delta t^2 s(x, t)$ is not an exact model of the inhomogeneous wave Eq. (A6.1.1). Figure A6.1.2 shows why this is so. For $u = 1$, g vanishes at half the points on the range $0 \leq |x/\Delta x| \leq u(t/\Delta t)$ so that the sampling frequency of the source is effectively cut in half.

Whatever the value of u , $g(\chi\Delta x, \tau\Delta t) \neq G(\chi\Delta x, \tau\Delta t)$, so g is not just a sampled version of G . For this reason, we distinguish it with a different symbol and name.

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Chapter 7

FDTD Algorithms to Solve the Wave Equation in Two and Three Dimensions

We now proceed to extend the 1D FDTD methodologies developed in Chapters 5 and 6 to two and three dimensions. With a few modifications and complications, the process is straightforward.

Topics:

- Standard and nonstandard FDTD and their errors
- The computational boundary and the nonstandard Mur algorithm
- Green's function solutions and the discrete Green's function methodology
- The fuzzy grid representation
- The scattered field and its nonstandard FDTD model
- Validation by Mie scattering
- Detailed stability analyses

7.1 The Homogeneous Wave Equation

In two and three dimensions, the homogeneous wave equation is

$$(\partial_t^2 - v^2 \nabla^2) \psi(\mathbf{x}, t) = 0, \quad (7.1)$$

where $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$, and $\mathbf{x} = (x, y, z)$.

In unbounded free space, a general solution is a waveform propagating in the $\pm \hat{\mathbf{k}}$ direction, given by

$$\begin{aligned} \psi(x, t) &= f(\mathbf{k} \cdot \mathbf{x} \mp \omega t) \\ &= f(k[\hat{\mathbf{k}} \cdot \mathbf{x} \mp vt]), \end{aligned} \quad (7.2)$$

where $\hat{\mathbf{k}}$ is a unit vector, $\mathbf{k} = k\hat{\mathbf{k}}$, $k = |\mathbf{k}|$, $\omega = \nu k$, and f is an arbitrary function. Monochromatic solutions are infinite plane waves of the form

$$\phi_{\mathbf{k}}(\mathbf{x}, t) = e^{i(\mathbf{k} \cdot \mathbf{x} \mp \omega t)}, \quad (7.3a)$$

or

$$\phi_{\mathbf{k}}(\mathbf{x}, t) = e^{i(\omega t \mp \mathbf{k} \cdot \mathbf{x})}. \quad (7.3b)$$

Note 7.1

When ∇^2 is expressed in cylindrical or spherical coordinates, the solutions are expressed in terms of cylindrical or spherical Bessel functions (see Appendix 10.1), but these can be expressed as superpositions of plane waves.

Boundary conditions at media interfaces

The boundary conditions at media interfaces can be generalized from one dimension into two and three by considering waves propagating normally to the interface (see Fig. 7.1). The boundary conditions given by Eq. (4.24) become

$$\psi_1(\mathbf{x}_B, t) = \psi_2(\mathbf{x}_B, t), \quad (7.4a)$$

$$\hat{\nu} \cdot \nabla \psi_1(\mathbf{x}_B, t) = \hat{\nu} \cdot \nabla \psi_2(\mathbf{x}_B, t), \quad (7.4b)$$

where $\hat{\nu}$ is a unit vector normal to the boundary at $\mathbf{x}_B$, and ψ_1 and ψ_2 are the fields on either side of the boundary.

In two and three dimensions, these boundary conditions are much more difficult to satisfy than in one dimension, and it is thus very difficult to find analytical solutions except when the boundaries have a high degree of symmetry; otherwise, numerical methods must be employed. The advantage of the FDTD methodology is that the boundary conditions are enforced implicitly as the algorithm is iterated.

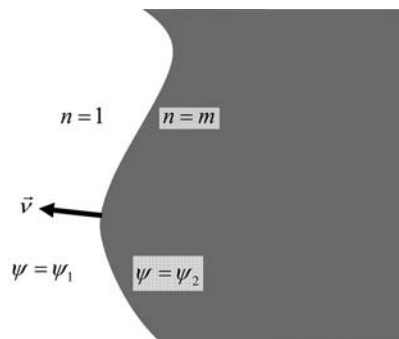


Figure 7.1 Curved interface between two media.

7.2 FDTD for the Homogeneous Wave Equation

7.2.1 Standard FDTD

We now extend the standard (S) and nonstandard (NS) FDTD methodology to two and three dimensions.

The S-FD model of the wave equation is derived with the substitutions

$$\partial_t^2 \rightarrow \frac{d_t^2}{\Delta t^2}, \quad (7.5a)$$

$$\nabla^2 \rightarrow \frac{\mathbf{d}^2}{h^2}, \quad (7.5b)$$

where $\mathbf{d}^2$ is defined in Section 1.3. The S-FD model is

$$(d_t^2 - u^2 \mathbf{d}^2)\psi(\mathbf{x}, t) = 0, \quad (7.6)$$

where

$$u = \frac{v\Delta t}{h}, \quad (7.7)$$

and $h = \Delta x = \Delta y = \Delta z$. Expanding $d_t^2\psi$ and solving for $\psi(\mathbf{x}, t + \Delta t)$ gives the S-FDTD algorithm

$$\psi(\mathbf{x}, t + \Delta t) = -\psi(\mathbf{x}, t - \Delta t) + (2 + u^2 \mathbf{d}^2)\psi(\mathbf{x}, t). \quad (7.8)$$

Error of S-FDTD

Defining the error ε_S of the S-FD model with respect to an infinite plane wave by

$$(d_t^2 - u^2 \mathbf{d}^2)e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} = \varepsilon_S e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}, \quad (7.9)$$

and using $\omega\Delta t = ukh$ then expanding in a Taylor series about $kh = 0$, we find that

$$\begin{aligned} \varepsilon_S &= 4\{-\sin^2(ukh/2) + u^2[\sin^2(kh \cos \theta/2) + \sin^2(kh \sin \theta/2)]\} \\ &= -\frac{1}{3}\left(\frac{kh}{2}\right)^4 u^2[3 + \cos(4\theta) - 4u^2] + \cdots \end{aligned} \quad (7.10)$$

in two dimensions, where $\mathbf{k} = k(\cos\theta, \sin\theta)$. In three dimensions, $\mathbf{k} = k(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, and we also find that

$$\varepsilon_S \sim \left(\frac{kh}{2}\right)^4. \quad (7.11)$$

The complete expression for ε_S in three dimensions is a long, complicated function of θ and φ , which we omit.

Numerical stability and Nyquist limits for S-FDTD

In $d =$ one, two, and three dimensions, the greatest distance between adjacent grid points is $h\sqrt{d}$; thus, for wavelength λ , the Nyquist limit gives the constraint

$$\frac{\lambda}{h} > 2\sqrt{d}. \quad (7.12)$$

As shown in Appendix 7.1, the condition for numerical stability is

$$\frac{v\Delta t}{h} \leq \frac{1}{\sqrt{d}}. \quad (7.13)$$

Combining Eqs. (7.12) and (7.13), the time discretization for a wave of period T is constrained by

$$\frac{T}{\Delta t} > 2d, \quad (7.14)$$

where we have used $v = \lambda/T$.

Devil in the details

When S-FDTD is used in combination with the standard Mur absorbing boundary condition (see Section 7.5), the practical stability limits are $v\Delta t/h \leq 1, 0.67, 0.45$ in one, two, and three dimensions, respectively.

7.2.2 Nonstandard FDTD

The NS-FD model is obtained from the S-FD model with the substitutions $v\Delta t/h \rightarrow \tilde{v}$ and $\mathbf{d}^2 \rightarrow \tilde{\mathbf{d}}^2$, where

$$\tilde{v} = \frac{\sin(\omega\Delta t/2)}{\sin(kh/2)}, \quad (7.15)$$

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \left(\frac{1}{6} + \frac{(kh)^2}{180}\right)(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \frac{1}{30} d_x^2 d_y^2 d_z^2. \quad (7.16)$$

(See Section 1.4 for the derivation of $\tilde{\mathbf{d}}^2$.)

Note 7.2

$\tilde{\mathbf{d}}^2 = \tilde{\mathbf{d}}^2(nk_0)$ is a function the local wavenumber $k = nk_0$ (n is the local refractive index). Evaluating $(k^2 h^2 / 180)(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) e^{i\mathbf{k} \cdot \mathbf{x}}$ for $k = nk_0$ and $k = k_0$, and computing the magnitude of the difference, we find that it is small for typical FDTD parameters and for most physically

realizable values of n . It is thus often an excellent approximation to take $k = k_0$ everywhere and define $\tilde{\mathbf{d}}^2 = \tilde{\mathbf{d}}^2(k_0)$ over the entire computational domain.

The NS-FD model becomes

$$\left(d_t^2 - \tilde{v}^2 \tilde{\mathbf{d}}^2\right) \psi(\mathbf{x}, t) = 0, \quad (7.17)$$

and the corresponding NS-FDTD algorithm is

$$\psi(\mathbf{x}, t + \Delta t) = -\psi(\mathbf{x}, t - \Delta t) + \left(2 + \tilde{v}^2 \tilde{\mathbf{d}}^2\right) \psi(\mathbf{x}, t). \quad (7.18)$$

Error of NS-FDTD

Defining the error ϵ_{NS} of the NS-FD model by

$$\left(d_t^2 - \tilde{v}^2 \tilde{\mathbf{d}}^2\right) e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} = \epsilon_{\text{NS}} e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}, \quad (7.19)$$

and taking $\tilde{v} = \sin(ukh/2)/\sin(kh/2)$, where $u = \omega\Delta t/kh$, then expanding in a Taylor series about $kh = 0$ in two dimensions, we find that

$$\begin{aligned} \epsilon_{\text{NS}} &= 4 \left\{ -\sin^2(ukh/2) + \frac{\sin^2(ukh/2)}{\sin^2(kh/2)} [\sin^2(kh \cos \theta/2) + \sin^2(kh \sin \theta/2)] \right\} \\ &\quad - 16 \frac{\sin^2(\omega\Delta t/2)}{\sin^2(kh/2)} \sin^2(kh \cos \theta/2) \sin^2(kh \sin \theta/2) \\ &= \frac{1}{1890} \left(\frac{kh}{2}\right)^8 u^2 \sin^2(2\theta) [12 - 5 \sin^2(2\theta)] + \cdots. \end{aligned} \quad (7.20)$$

Note 7.3

$\epsilon_{\text{NS}} = 0$ exactly at $\theta = 0, \pm\pi/2$, and π . Thus, the error vanishes with respect to infinite plane waves propagating along the principle axes.

A similar result is obtained in three dimensions (it is quite complicated, so we omit the expression).

As explained in Chapter 5, Note 5.1, in NS-FDTD, the error vanishes for all ω and k that satisfy $\sin(\omega\Delta t/2)/\sin(kh/2) = \tilde{v}$ in a uniform medium. As discussed in Section 6.5.4 (see Fig. 6.6), the effective refractive index $\tilde{n}_s$ changes with frequency. In a calculation with multiple refractive indices, to the extent that a variation of $\tilde{\mathbf{d}}^2$ with n is weak, the error is small (some correction for variation of $\tilde{n}_s$ with frequency is possible). Often it is sufficient to use the $\tilde{\mathbf{d}}^2$ operator and $\tilde{n}_s$ value corresponding to the highest frequency.

It is interesting to evaluate the error of the NS-FD model using $\gamma_1 = 1/6$. Let us set

$$\mathbf{d}^2 \rightarrow \tilde{\mathbf{d}}_{1/6}^2 = \mathbf{d}^2 + \frac{1}{6}(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \frac{1}{30} d_x^2 d_y^2 d_z^2. \quad (7.21)$$

$\tilde{\mathbf{d}}_{1/6}^2$ is completely independent of k , but the error of the NS-FD model with $\tilde{\mathbf{d}}_{1/6}^2$ is somewhat larger:

$$\varepsilon_{\text{NS}}(\gamma = 1/6) = \frac{4}{45} \left(\frac{kh}{2} \right)^6 u^2 \sin^2(2\theta) + \dots \quad (7.22)$$

Since $\tilde{\mathbf{d}}_{1/6}^2$ is wavelength independent, it is useful in the discrete Green's function methodology described in Section 7.8.

Error and computational cost: S-FDTD versus NS-FDTD

The error of S-FDTD is $\varepsilon_S \sim (h/\lambda)^4$, and the computational cost, which is proportional to the number of space–time points that must be computed, is $C \sim (\lambda/h)^{d+1}$, where d is the number of spatial dimensions, and λ is the wavelength. Because Δt must be scaled down with h in order to maintain numerical stability, $\Delta t \sim h$. In one dimension, putting $h \rightarrow h/2$ (which implies that $\varepsilon_S \rightarrow \varepsilon_S/16$) and $C \rightarrow 4C$ but in three dimensions, $C \rightarrow 16C$. On the other hand, the NS-FDTD algorithm is exact in one dimension, and in two and three dimensions, $\varepsilon_{\text{NS}} \sim (h/\lambda)^8$, and $h \rightarrow h/2$, which implies that $\varepsilon_{\text{NS}} \rightarrow \varepsilon_{\text{NS}}/256$. Although, strictly speaking, these considerations only apply to propagation in an unbounded uniform medium, NS-FDTD is much more accurate on actual problems. In Section 7.4.4 we compare the error of S- and NS-FDTD for a Mie scattering problem that has a known analytic solution, and find that NS-FDTD has a much lower error.

Numerical Stability for NS-FDTD

As shown in Appendix 7.1 (also see Note A7.5.1), the condition for numerical stability is

$$\tilde{v} \leq 1 \quad \text{in one dimension.} \quad (7.23a)$$

In two dimensions, we find the condition $\tilde{v} \leq \sqrt{3}/2 \cong 0.86$; however, with the Mur absorbing boundary (see Section 7.5), a practical limit, which we have verified in long computations, is

$$\tilde{v} \leq 0.80 \quad \text{in two dimensions.} \quad (7.23b)$$

Similarly, in three dimensions, we find that $\tilde{v} \leq \sqrt{15/23} \cong 0.80$, and with the Mur absorbing boundary, the practical limit is

$$\tilde{v} \leq 0.70 \quad \text{in three dimensions.} \quad (7.23c)$$

From Eq. (7.23) we can extract the maximum possible time step for a given frequency, but in a practical NS-FDTD program we fix $\tilde{v}$ and then choose the wavelengths and frequencies that satisfy Eq. (7.15). In this way, the NS-FDTD error is low for all wavelengths and frequencies related by Eq. (7.15).

These limits are also valid with the nonstandard Mur absorbing boundary condition (Section 7.5).

7.2.3 FDTD for the damped wave equation

The damped wave equation in two and three dimensions is

$$(\partial_t^2 + 2\alpha\partial_t - v^2\nabla^2)\psi(\mathbf{x}, t) = 0. \quad (7.24)$$

The results of Chapter 5 can be straightforwardly carried over to two and three dimensions. Replacing d_x^2 by $\mathbf{d}^2$, the SC-FDTD algorithm of Eq. (5.23) becomes the following:

S-FDTD:

$$\psi(\mathbf{x}, t + \Delta t) = -\left(\frac{1 - \alpha\Delta t}{1 + \alpha\Delta t}\right)\psi(\mathbf{x}, t - \Delta t) + \frac{1}{1 + \alpha\Delta t}(2 + u^2\mathbf{d}^2)\psi(\mathbf{x}, t). \quad (7.25)$$

The 1D NS-FDTD algorithm [Eq. (5.32)] generalizes to two and three dimensions with the substitutions $\mathbf{d}^2 \rightarrow \tilde{\mathbf{d}}^2$, $u^2 \rightarrow \tilde{v}^2$, and $\alpha\Delta t \rightarrow \tilde{\alpha}'$ in Eq. (7.25) to become the following:

NS-FDTD (complex wavenumber solution):

$$\psi(\mathbf{x}, t + \Delta t) = -\left(\frac{1 - \tilde{\alpha}'}{1 + \tilde{\alpha}'}\right)\psi(\mathbf{x}, t - \Delta t) + \frac{1}{1 + \tilde{\alpha}'}(2 + \tilde{v}^2\tilde{\mathbf{d}}^2)\psi(\mathbf{x}, t), \quad (7.26)$$

where

$$\tilde{v}^2 = \frac{2 \sin^2(\omega\Delta t/2)}{1 - \cos(k'_r h) \cosh(k'_i h)}, \quad (7.27)$$

$$\tilde{\alpha}' = \frac{-\tilde{v}^2 \sin(k'_r h) \sinh(k'_i h)}{\sin(\omega\Delta t)}, \quad (7.28)$$

$k' = k\sqrt{1 - 2i\alpha/\omega} = k'_r + ik'_i$ is the complex wavenumber, and $\omega = kv$.

7.3 Wave Equation with a Source

The wave equation with a source is

$$(\partial_t^2 - v^2\nabla^2)\psi(\mathbf{x}, t) = s(\mathbf{x}, t). \quad (7.29)$$

In the absence boundaries, Eq. (7.29) describes waves emanating from a source in a uniform medium. Following the discussion of Section 4.5, we take the initial conditions to be

$$\psi(\mathbf{x}, t) = 0 \quad \text{for } t < 0, \quad (7.30a)$$

$$\partial_t \psi(\mathbf{x}, t) = 0 \quad \text{for } t < 0, \quad (7.30b)$$

and then make the substitution, $s(\mathbf{x}, t) \rightarrow \Theta(t)s(\mathbf{x}, t)$, where Θ is the step function (see Appendix 3.4). The solution of Eq. (7.29) can be expressed in terms of a Green's function G by

$$\psi(\mathbf{x}, t) = \int_{-\infty}^{\infty} dt' \int_{\mathbf{x}' \in \mathbb{R}^3} d^3 \mathbf{x}' G(\mathbf{x}, t; \mathbf{x}', t') s(\mathbf{x}', t'), \quad (7.31)$$

where $\mathbb{R}^3$ denotes all (x, y, z) in a real vector space, and $d^3 \mathbf{x}' = dx' dy' dz'$.

The Green's function satisfies

$$(\partial_t^2 - v^2 \nabla^2) G(\mathbf{x}, t; \mathbf{x}', t') = \Delta(\mathbf{x} - \mathbf{x}') \Delta(t - t'), \quad (7.32)$$

where $\delta(\mathbf{x} - \mathbf{x}') = \delta(x - x')\delta(y - y')\delta(z - z')$. Physically, it is the field produced by a point source located at $\mathbf{x}' = (x', y', z')$ with time dependence $\delta(t - t')$. On physical (and mathematical) grounds, we can assume that in an unbounded uniform medium,

$$G(\mathbf{x}, t; \mathbf{x}', t') = G(\mathbf{x} - \mathbf{x}', t - t'). \quad (7.33)$$

In two dimensions,

$$G(\mathbf{x} - \mathbf{x}', t - t') = \frac{1}{2\pi v} \frac{\Theta[v(t - t') - |\mathbf{x} - \mathbf{x}'|]}{\sqrt{v^2(t - t')^2 - |\mathbf{x} - \mathbf{x}'|^2}}, \quad (7.34)$$

and in three dimensions

$$G(\mathbf{x} - \mathbf{x}', t - t') = \frac{\Delta[v(t - t') - |\mathbf{x} - \mathbf{x}'|]}{4\pi v^3 |\mathbf{x} - \mathbf{x}'|}, \quad (7.35)$$

as shown in Refs. 1 and 2.

The solution of Eq. (7.29) in two dimensions is thus

$$\psi(\mathbf{x}, t) = \frac{1}{2\pi v} \int d^2 \mathbf{x}' \int_0^{t - |\mathbf{x} - \mathbf{x}'|/v} dt' \frac{s(\mathbf{x}', t')}{\sqrt{v^2(t - t')^2 - |\mathbf{x} - \mathbf{x}'|^2}}, \quad (7.36)$$

and in three dimensions is

$$\psi(\mathbf{x}, t) = \frac{1}{4\pi v^3} \int d^3 \mathbf{x}' \int_0^{t-|\mathbf{x}-\mathbf{x}'|/v} dt' \frac{s(\mathbf{x}', t-|\mathbf{x}-\mathbf{x}'|/v)}{|\mathbf{x}-\mathbf{x}'|}. \quad (7.37)$$

It is interesting to note that the solution is much simpler in three dimensions than in two.

For example, let us compute the field due to a point source located at the origin of the form

$$s(\mathbf{x}, t) = \Theta(t) \sigma(t) \Delta(\mathbf{x}). \quad (7.38)$$

Point source in two dimensions

Inserting source Eq. (7.38) into the 2D solution of Eq. (7.36) gives

$$\psi(\mathbf{x}, t) = \frac{\Theta(vt - r)}{2\pi v^2} \int_0^{t-r/v} dt' \frac{\sigma(t')}{\sqrt{(t-t')^2 - r^2/v^2}}, \quad (7.39)$$

where $r = |\mathbf{x}|$. Although the factor $\Theta[v(t - t') - r]$ determines the upper integration limit, we retain it outside the integral to ensure causality. Because the source turns on at $t = 0$ and waves travel with velocity v , $\psi(\mathbf{x}, t) = 0$ for $|\mathbf{x}| > vt$. Defining $\tau = t - t'$ and $\tau' = vt/r$, which implies that $d\tau = rd\tau'/v$, the integral can be transformed as

$$\begin{aligned} \int_0^{t-r/v} dt' \frac{\sigma(t')}{\sqrt{(t-t')^2 - r^2/v^2}} &= \int_{r/v}^t d\tau \frac{\sigma(t-\tau)}{\sqrt{\tau^2 - r^2/v^2}} \\ &= \int_1^{vt/r} d\tau' \frac{\sigma(t-\tau' r/v)}{\sqrt{\tau'^2 - 1}}. \end{aligned} \quad (7.40)$$

Finally, defining $\tau' = \cosh \tau''$, which implies that $d\tau' = d\tau'' \sinh \tau''$, and using the identity $\cosh^2 x - \sinh^2 x = 1$ and the fact that $\cosh^{-1}(1) = 0$, we obtain

$$\psi(\mathbf{x}, t) = \frac{\Theta(vt - r)}{2\pi v^2} \int_0^{\cosh^{-1}(vt/r)} d\tau \sigma(t - r \cosh \tau/v). \quad (7.41)$$

Equation (7.41) is useful for numerical computations.

Note 7.4

Since $y = \cosh(\pm x)$, $\cosh^{-1} y = \ln [y \pm \sqrt{y^2 - 1}]$, and $vt/r > 1$, we take $\cosh^{-1} y = \ln [y + \sqrt{y^2 - 1}]$ in the upper integration limit in Eq. (7.41).

Harmonic time dependence

Taking $\sigma(t) = e^{-i\omega t}$, where $\nu = \omega/k$, Eq. (7.41) becomes

$$\begin{aligned}\psi(\mathbf{x}, t) &= \frac{\Theta(\nu t - r)}{2\pi\nu^2} e^{-i\omega t} \int_1^{\nu t/r} \frac{e^{ikr\tau} d\tau}{\sqrt{\tau^2 - 1}} \\ &= \frac{\Theta(\nu t - r)}{2\pi\nu^2} e^{-i\omega t} \int_0^{\cosh^{-1}(\nu t/r)} d\tau e^{ikr \cosh \tau}.\end{aligned}\quad (7.42)$$

Using the fact that

$$i\frac{\pi}{2} H_0^{(1)}(x) = \int_1^\infty d\tau \frac{e^{ix\tau}}{\sqrt{\tau^2 - 1}} \quad (7.43)$$

in the limit $t \rightarrow \infty$ at fixed r , we have

$$\lim_{t \rightarrow \infty} \psi(\mathbf{x}, t) = \frac{i}{4\nu^2} e^{-i\omega t} H_0^{(1)}(kr). \quad (7.44)$$

An outgoing radially symmetric solution to the homogeneous wave equation without boundary or initial conditions (see Appendix 7.1) is

$$\varphi(r, t) = e^{-i\omega t} H_0^{(1)}(kr), \quad (7.45)$$

so Eq. (7.44) tells us that long after the source has been turned on, Eq. (7.42) converges to the form of the steady state solution of Eq. (7.45).

We can gain further insight into the properties of solution Eq. (7.45) by examining its far-field behavior. The asymptotic expansion of $H_0^{(1)}(x)$, valid at large x , is

$$H_0^{(1)}(x) = \sqrt{\frac{2}{\pi x}} e^{i(x - \pi/4)} + \dots \quad (7.46)$$

At large r but with $\nu t/r \rightarrow \infty$, we thus have

$$\psi(\mathbf{x}, t) = \frac{(1+i)}{4\nu^2 \sqrt{\pi}} \frac{e^{i(kr - \omega t)}}{\sqrt{r}}. \quad (7.47)$$

This tells us that intensity falls off as $1/r$.

Harmonic point source in three dimensions

Taking $\sigma(t) = e^{-i\omega t}$ in Eq. (7.38) and evaluating Eq. (7.37), we find that

$$\psi(\mathbf{x}, t) = \frac{1}{4\pi v^3 r} e^{i(kr - \omega t)}, \quad (7.48)$$

where $r = |\mathbf{x}|$, and $\omega = kv$. Now the intensity falls off as $1/r^2$.

Dimensionality and intensity falloff

The intensity of the wave field is proportional to $|\psi(\mathbf{x}, t)|^2$. Comparing Eqs. (4.58), (7.47), and (7.48), we see that in d dimensions, intensity falls off as $1/r^{d-1}$ from a point source. This can be heuristically deduced by considering the amount of energy per unit time crossing a point boundary in one dimension, a circular boundary of circumference $2\pi r$ in two dimensions, and a spherical surface of area $2\pi r^2$ in three dimensions centered on the point source. The fall-off of intensity with distance from the source thus tells us the dimensionality of the space. If, for example, we lived in a space with a compact fourth spatial dimension, gravitational strength might fall off as $1/r^3$ at short distances. Experiments to accurately measure the variation of gravitational attraction with distance are underway—see the current physics literature—and might yield insight into the dimensionality and topology of the space in which we live.

Standard and nonstandard FDTD for the inhomogeneous wave equation

The 1D formulation can be directly generalized to two and three dimensions. Adding a source, the S-FDTD algorithm of Eq. (7.8) becomes

$$\psi(\mathbf{x}, t + \Delta t) = -\psi(\mathbf{x}, t - \Delta t) + (2 + u^2 \mathbf{d}^2) \psi(\mathbf{x}, t) + \Delta t^2 s(\mathbf{x}, t). \quad (7.49)$$

Since any solution of the wave equation can be expanded as a superposition of infinite plane waves, the 1D NS source model [Eq. (5.52)] is valid in two and three dimensions for a source with harmonic time dependence. Thus, Eq. (7.18) becomes

$$\psi(\mathbf{x}, t + \Delta t) = -\psi(\mathbf{x}, t - \Delta t) + (2 + \tilde{v}^2 \tilde{\mathbf{d}}^2) \psi(\mathbf{x}, t) + \tilde{s}(\mathbf{x}, t), \quad (7.50)$$

where $\tilde{s}(\mathbf{x}, t) = \tilde{A}s(\mathbf{x}, t)$, and $\tilde{A}$, given by Eq. (5.51), is

$$\tilde{A} = \frac{2}{v^2 k} \frac{\sin^2(\omega \Delta t / 2)}{\tan(kh/2)}. \quad (7.51)$$

7.4 The Scattered Field

7.4.1 Analytic solution

We now extend the 1D development of Sections 4.5 and 6.5 to two and three dimensions. Reiterating that discussion, an incident field ψ_0 impinges on a scatterer of refractive index n_s relative to the medium in which it is immersed. The wave equation to be solved is

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \nabla^2\right) \psi(\mathbf{x}, t) = 0, \quad (7.52)$$

where $n = n_s$ inside the scatterer, and $n = 1$ outside the scatterer. On the boundary between the scatterer and the ambient medium, ψ must satisfy the boundary conditions given by Eq. (7.4). The solution of Eq. (7.52) can be decomposed into two parts in the form

$$\psi = \psi_0 + \psi_s, \quad (7.53)$$

where ψ_s is the scattered field. The incident field propagates as if there were no scatterer and obeys

$$(\partial_t^2 - v_0^2 \nabla^2) \psi_0(\mathbf{x}, t) = 0. \quad (7.54)$$

Subtracting Eq. (7.54) from Eq. (7.52) yields the wave equation for the scattered field:

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \nabla^2\right) \psi_s(\mathbf{x}, t) = s_0(\mathbf{x}, t), \quad (7.55)$$

where s_0 is the source of the scattered field, and

$$\begin{aligned} s_0(\mathbf{x}, t) &= -\left(\frac{n^2 - 1}{n^2}\right) \partial_t^2 \psi_0(\mathbf{x}, t) \quad \text{for } \mathbf{x} \in \mathbf{S}, \\ &= 0 \quad \text{for } \mathbf{x} \notin \mathbf{S}, \end{aligned} \quad (7.56)$$

where $\mathbf{S}$ is the set of points inside the scatterer. Following Section 4.7, we impose the initial conditions

$$\psi_s(\mathbf{x}, t) = 0 \quad \text{for } t < 0, \quad (7.57a)$$

$$\partial_t \psi_s(\mathbf{x}, t) = 0 \quad \text{for } t < 0. \quad (7.57b)$$

Thus, we replace $s_0(\mathbf{x}, t)$ with $\Theta(t)s_0(\mathbf{x}, t)$ so that Eq. (7.55) becomes

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \nabla^2\right) \psi_s(\mathbf{x}, t) = \Theta(t)s_0(\mathbf{x}, t). \quad (7.58)$$

The formal solution of Eq. (7.58) is given in terms of a Green's function $G(\mathbf{x}, t; \mathbf{x}', t')$ that satisfies the boundary conditions given by Eq. (7.4) and the initial conditions given by Eq. (7.57) with respect to $\mathbf{x}$ and t :

$$\psi_s(\mathbf{x}, t) = \Theta(t) \int_0^\infty dt' \sigma(t') \int_{\mathbf{x}' \in S} d^3\mathbf{x}' G(\mathbf{x}, \mathbf{x}', t - t') s_0(\mathbf{x}', t'). \quad (7.59)$$

Here we take $G(\mathbf{x}, t; \mathbf{x}', t') = G(\mathbf{x}, \mathbf{x}', t - t')$ but make no assumption on the form of the spatial dependence of G . The time integration begins at $t' = 0$ because the source turns on at $t = 0$. It need not be carried out to $t' = \infty$, but in the absence of information about the propagation velocity from $\mathbf{x}'$ to $\mathbf{x}$, we leave this limit in place. Usually the appropriate Green's function is difficult, if not impossible, to find.

This model differs from that used to compute analytic solutions (see Note 4.5), such as those given by Mie theory (see Appendix 7.2), where the incident field is assumed to be present at $t = -\infty$. On the other hand, the solution given by Eq. (7.58), which gives the time evolution of ψ_s after the source is turned on, might be expected to differ from the scattered field computed using Mie theory. However, in practice, ψ_s converges to the Mie result for sufficiently large t , and it usually converges rather quickly, except in the case of resonances, such as whispering gallery modes (see Appendix 10.3 and Section 11.2), where a large number of time steps must be computed.

In deriving analytic solutions to the scattering problem, one often takes ψ_0 to be an infinite plane wave $\varphi_0(\mathbf{x}, t) = e^{i(\mathbf{k}_0 \cdot \mathbf{x} - \omega t)}$ such that

$$\begin{aligned} s_0(\mathbf{x}, t) &= \omega^2 \left(\frac{n_s^2 - 1}{n_s^2} \right) \varphi_0(\mathbf{x}, t) \quad \text{for } \mathbf{x} \in S, \\ &= 0 \quad \text{for } \mathbf{x} \notin S. \end{aligned} \quad (7.60)$$

7.4.2 The standard finite difference model

The derivatives of the scattered-field wave equation are replaced by S-FD expressions, and the source of the scattered field is turned on slowly: $s_0 \rightarrow \Theta_g s_0$, where $\Theta_g(t) = \Theta(t)[1 - e^{-(t/\tau)^2}]$. The S-FD model becomes

$$\left(d_t^2 - \frac{v_0^2 \Delta t^2}{n^2 h^2} \mathbf{d}^2 \right) \psi_s(\mathbf{x}, t) = \Delta t^2 \Theta_g(t) s_0(\mathbf{x}, t), \quad (7.61)$$

and the S-FDTD algorithm becomes

$$\psi_s(\mathbf{x}, t + \Delta t) = -\psi_s(\mathbf{x}, t - \Delta t) + \left(2 + \frac{v_0^2 \Delta t^2}{n^2 h^2} \mathbf{d}^2 \right) \psi_s(\mathbf{x}, t) + \Delta t^2 \Theta_g(t) s_0(\mathbf{x}, t). \quad (7.62)$$

The computation is initialized by setting $\psi_s(\mathbf{x}, -\Delta t) = \psi_s(\mathbf{x}, 0) = 0$ and turning on the source at $t = 0$. The boundary conditions on the scatterer are automatically satisfied as the iteration of Eq. (7.62) proceeds.

7.4.3 Nonstandard FDTD

Taking the incident field to be $\psi_0 = e^{i(\mathbf{k}_0 \cdot \mathbf{x} - \omega t)}$ and generalizing the 1D development of Section 4.7, the NS-FD model is obtained from the S-FD model with the substitutions $v_0 \Delta t / h \rightarrow \tilde{v}_0 = \sin(\omega \Delta t / 2) / \sin(k_0 h / 2)$ and $n \rightarrow \tilde{n} = \sin(n k_0 h / 2) / \sin(k_0 h / 2)$ to obtain

$$\left[d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} \tilde{\mathbf{d}}(n)^2 \right] \psi(\mathbf{x}, t) = 0, \quad (7.63)$$

where we now explicitly include the dependence of $\tilde{\mathbf{d}}^2$ on $k = n k_0$ (see Section 1.4). In the ambient medium, where $n = \tilde{n} = 1$ and for $\mathbf{k}_0 = (k_{0x}, k_{0y}, k_{0z})$, the incident field propagates according to the exact NS-FD model:

$$\left[d_t^2 - \frac{\sin^2(\omega \Delta t / 2)}{\sum_{i=x,y,z} \sin^2(k_{0i} h / 2)} \mathbf{d}^2 \right] \psi_0(\mathbf{x}, t) = 0. \quad (7.64)$$

Because this model is exact,

$$\begin{aligned} \frac{\sin^2(\omega \Delta t / 2)}{\sum_{i=x,y,z} \sin^2(k_{0i} h / 2)} \mathbf{d}^2 \varphi_0(\mathbf{x}, t) &= d_t^2 \psi_0(\mathbf{x}, t) \\ &= -4 \sin^2(\omega \Delta t / 2) \psi_0(\mathbf{x}, t) \end{aligned} \quad (7.65)$$

is an identity. Subtracting Eq. (7.64) from Eq. (7.63), and using $\psi_s = \psi - \psi_0$ and identity Eq. (7.65), we obtain the NS-FD model of the scattered field,

$$\left[d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} \tilde{\mathbf{d}}^2(n) \right] \psi_s(\mathbf{x}, t) = \Theta_g(t) \tilde{s}_0(\mathbf{x}, t), \quad (7.66)$$

where

$$\begin{aligned} \tilde{s}_0(\mathbf{x}, t) &= \left[\frac{\tilde{v}_0^2}{\tilde{n}_s^2} \tilde{\mathbf{d}}^2(n_s) + 4 \sin^2(\omega \Delta t / 2) \right] \psi_0(\mathbf{x}, t) \quad \text{for } \mathbf{x} \in \mathbf{S}, \\ &= 0 \quad \text{for } \mathbf{x} \notin \mathbf{S}, \end{aligned} \quad (7.67)$$

and Θ_g is inserted to slowly turn on the source term.

Now we define $\tilde{\mathbf{d}}^2(n_s) - \tilde{\mathbf{d}}^2(1) = \Delta \tilde{\mathbf{d}}^2$. Because $\tilde{v}_0^2 \tilde{\mathbf{d}}^2(1) \psi_0 = -4 \sin^2(\omega \Delta t / 2) \psi_0$ is an excellent approximation, we can rewrite the source term as

$$\tilde{s}_0(\mathbf{x}, t) = 4 \sin^2(\omega \Delta t / 2) \left(\frac{\tilde{n}_s^2 - 1}{\tilde{n}_s^2} \right) \psi_0(\mathbf{x}, t) + \frac{\tilde{v}_0^2}{\tilde{n}_s^2} \Delta \tilde{\mathbf{d}}^2 \psi_0(\mathbf{x}, t) \quad \text{for } \mathbf{x} \in \mathbf{S}. \quad (7.68)$$

Writing $\tilde{s}_0 = \tilde{s}_1 + \tilde{s}_2$, where $\tilde{s}_1 = 4 \sin^2(\omega \Delta t / 2) [(\tilde{n}_s^2 - 1) / \tilde{n}_s^2] \psi_0$, and $\tilde{s}_2 = (\tilde{v}_0^2 / \tilde{n}_s^2) \Delta \tilde{\mathbf{d}}^2 \psi_0$, we compare the amplitudes of $\tilde{s}_1$ and $\tilde{s}_2$. Computing $\Delta \tilde{\mathbf{d}}^2$, we find that

$$\Delta \tilde{\mathbf{d}}^2 = \Delta \gamma_1 (d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2), \quad (7.69)$$

where $\gamma_1(n) = 1/6 + (nk_0h)^2/180$, and

$$\begin{aligned} \Delta \gamma_1 &= \gamma(n_s) - \gamma(1) \\ &= \frac{(n_s^2 - 1)k_0^2 h^2}{180}. \end{aligned} \quad (7.70)$$

Because we always choose $k_0h \leq 1$,

$$\Delta \gamma_1 < \frac{n_s^2 - 1}{180}. \quad (7.71)$$

Thus,

$$\begin{aligned} \frac{\Delta \tilde{\mathbf{d}}^2 \psi_0}{\psi_0} &= \frac{4}{45} (n_s^2 - 1) \left[\sin^2(k_{0x}h/2) \sin^2(k_{0y}h/2) \right. \\ &\quad \left. + \sin^2(k_{0x}h/2) \sin^2(k_{0z}h/2) + \sin^2(k_{0y}h/2) \sin^2(k_{0z}h/2) \right]. \end{aligned} \quad (7.72)$$

If $\mathbf{k}_0$ lies along one of the principal (x , y , or z) axes, then $(d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) \psi_0 = 0$, and hence $\Delta \tilde{\mathbf{d}}^2 \psi_0 = 0$. When this is not the case, it can be shown that

$$\max[\sin^2(k_{0x}h/2) \sin^2(k_{0y}h/2)] = \sin^4(k_0h\sqrt{2}/4) \quad (7.73a)$$

in two dimensions, and

$$\begin{aligned} \max[\sin^2(k_{0x}h/2) \sin^2(k_{0y}h/2) + \sin^2(k_{0x}h/2) \sin^2(k_{0z}h/2) \\ + \sin^2(k_{0y}h/2) \sin^2(k_{0z}h/2)] = 3 \sin^4(k_0h\sqrt{3}/6) \end{aligned} \quad (7.73b)$$

in three dimensions. For $k_0h \leq 1$,

$$\sin^4(k_0h\sqrt{2}/4) \leq (k_0h\sqrt{2}/4)^4 = (k_0h)^4/64, \quad (7.74a)$$

$$3 \sin^4(k_0 h \sqrt{3}/6) \leq 3(k_0 h \sqrt{3}/6)^4 = (k_0 h)^4/48; \quad (7.74b)$$

thus,

$$\frac{\Delta \tilde{\mathbf{d}}^2 \varphi_0}{\varphi_0} \leq (n_s^2 - 1) \frac{(k_0 h)^4}{720} \quad \text{in two dimensions,} \quad (7.75a)$$

$$\frac{\Delta \tilde{\mathbf{d}}^2 \varphi_{k_0}}{\varphi_{k_0}} \leq (n_s^2 - 1) \frac{(k_0 h)^4}{540} \quad \text{in three dimensions.} \quad (7.75b)$$

Combining everything, we find that

$$\frac{\tilde{s}_2}{\tilde{s}_1} \leq \frac{1}{720} \left(\frac{n_s^2 - 1}{\tilde{n}_s^2 - 1} \right) (k_0 h)^2 \quad \text{in two dimensions,} \quad (7.76a)$$

$$\leq \frac{1}{540} \left(\frac{n_s^2 - 1}{\tilde{n}_s^2 - 1} \right) (k_0 h)^2 \quad \text{in three dimensions.} \quad (7.76b)$$

Because $(n_s^2 - 1)/(\tilde{n}_s^2 - 1) \sim 1$, $\tilde{s}_2$ either vanishes or is small compared to $\tilde{s}_1$, so we henceforth neglect it and take the source of the scattered field to be

$$\begin{aligned} \tilde{s}_0(\mathbf{x}, t) &= 4 \sin^2(\omega \Delta t/2) \left(\frac{\tilde{n}_s^2 - 1}{\tilde{n}_s^2} \right) \varphi_0(\mathbf{x}, t) \quad \text{for } \mathbf{x} \in \mathbf{S}, \\ &= 0 \quad \text{for } \mathbf{x} \notin \mathbf{S}. \end{aligned} \quad (7.77)$$

The NS-FDTD algorithm for the scattered field thus becomes

$$\begin{aligned} \psi_s(\mathbf{x}, t + \Delta t) &= -\psi_s(\mathbf{x}, t - \Delta t) + \left[2 + \frac{\tilde{v}_0^2}{\tilde{n}^2} \tilde{\mathbf{d}}^2(n) \right] \psi_s(\mathbf{x}, t) \\ &\quad + \Theta_g(t) \tilde{s}_0(\mathbf{x}, t), \end{aligned} \quad (7.78)$$

where $\tilde{s}_0$ is given by Eq. (7.77). As previously discussed, we can often put $\tilde{\mathbf{d}}^2(1)$ in place of $\tilde{\mathbf{d}}^2(n)$ everywhere.

7.5 Absorbing Boundary Condition

As we have seen in Chapter 6, unless the wave field vanishes or is periodic on the boundaries of the computational domain, an absorbing boundary condition (ABC) is required to mimic an infinite computational domain. In one dimension, there exists a perfect ABC, but in two and three dimensions, the better the ABC the more complicated and computationally intensive it becomes. Many ABCs are available, and ABC development is still a subject of active research.

We make no attempt to give an exhaustive review of ABCs but rather present an easy-to-implement, low-cost method that works reasonably well in many cases.

7.5.1 One-way wave equations

Unlike the 1D case, the wave equation in more than one dimension cannot be factored into two one-way wave equations without mathematical contrivance. For simplicity, first consider the 2D wave equation in the form

$$[d_t^2 - v^2(\partial_x^2 + \partial_y^2)]\psi(\mathbf{x}, t) = 0, \quad (7.79)$$

where $\mathbf{x} = (x, y)$ on the computational domain $(0 \leq x \leq b_x) \times (0 \leq y \leq b_y)$. Defining

$$P = \sqrt{\partial_t^2 - v^2\partial_y^2}, \quad (7.80)$$

Eq. (7.79) can be factored into

$$(P + v\partial_x)(P - v\partial_x)\psi(\mathbf{x}, t) = 0. \quad (7.81)$$

One-way wave equations with respect to propagation in the $\pm x$ directions are thus

$$(P \pm v\partial_x)\psi(\mathbf{x}, t) = 0. \quad (7.82)$$

Equation (7.82) is called the Engquist–Majda³ one-way wave equation. By analogy with the 1D case, where $(\partial_t \pm v\partial_x)f(x \mp vt) = 0$, we hope that

$$(P \pm v\partial_x)f(\mathbf{k} \bullet \mathbf{x} \mp \omega t) = 0, \quad (7.83)$$

where f is an arbitrary function, and $\mathbf{k} = k(\cos\theta, \sin\theta)$. Writing $P = \sqrt{P^2}$ and expanding it via the binomial theorem, we obtain

$$\begin{aligned} P &= \partial_t \sqrt{1 - \frac{v^2\partial_y^2}{\partial_t^2}} = \partial_t \left[1 - \frac{1}{2} \frac{v^2\partial_y^2}{\partial_t^2} + \cdots \right] \\ &\cong \partial_t - \frac{1}{2} \frac{v^2\partial_y^2}{\partial_t}. \end{aligned} \quad (7.84)$$

Boldly assuming (see Note 2.2) that Eq. (7.82) has the same solution as (or at least a solution in common with)

$$\partial_t(P \pm v\partial_x)\psi(\mathbf{x}, t) = 0, \quad (7.85)$$

and assuming that the product of operators ∂_t and P is $\partial_t P \cong \partial_t^2 - v^2\partial_y^2/2 + \cdots$, we obtain the approximate one-way wave equations:

$$\left(\partial_t^2 + v\partial_t\partial_x - \frac{1}{2}v^2\partial_y^2\right)\psi(x, y, t)|_{x=b_x} = 0, \quad (7.86a)$$

$$\left(\partial_t^2 - v\partial_t\partial_x - \frac{1}{2}v^2\partial_y^2\right)\psi(x, y, t)|_{x=0} = 0. \quad (7.86b)$$

Taking $\psi = f(\mathbf{k} \bullet \mathbf{x} \mp \omega t)$, the right sides of Eq. (7.86) would vanish if $f(\mathbf{k} \bullet \mathbf{x} \mp \omega t)$ were solutions. Instead,

$$\begin{aligned} \left(\partial_t^2 \pm v\partial_t\partial_x - \frac{1}{2}v^2\partial_y^2\right)f(\mathbf{k} \bullet \mathbf{x} \mp \omega t) &= \omega^2 \frac{f''(\mathbf{k} \bullet \mathbf{x} \mp \omega t)}{f(\mathbf{k} \bullet \mathbf{x} \mp \omega t)} \left(1 - \cos\theta - \frac{1}{2}\sin^2\theta\right) \\ &= \omega^2 \frac{f''(\mathbf{k} \bullet \mathbf{x} \mp \omega t)}{f(\mathbf{k} \bullet \mathbf{x} \mp \omega t)} \left(\frac{1}{8}\theta^4 - \frac{1}{48}\theta^6 + \dots\right). \end{aligned} \quad (7.87)$$

Although $f(\mathbf{k} \bullet \mathbf{x} \mp \omega t)$ are not solutions (except for the special case where $\theta = 0$), for $|\theta| < 1$, the reflection [which is proportional to the right side of Eq. (7.87)] is small provided that $\omega^2 f''/f$ is not too large.

With respect to propagation in the $\pm y$ directions, the Engquist–Majda one-way wave equations are

$$\left(\partial_t^2 + v\partial_t\partial_y - \frac{1}{2}v^2\partial_x^2\right)\psi(x, y, t)|_{y=b_y} = 0, \quad (7.88a)$$

$$\left(\partial_t^2 - v\partial_t\partial_y - \frac{1}{2}v^2\partial_x^2\right)\psi(x, y, t)|_{y=0} = 0. \quad (7.88b)$$

7.5.2 Standard finite difference model

From the Engquist–Majda one-way wave equations, we can derive an approximate ABC that is suitable for FDTD calculations. For simplicity, let us derive the S-FD model from Eq. (7.86a) for the $x = b_x$ boundary. Replacing derivatives with the FD expressions $\partial_t^2 \rightarrow d_t^2/\Delta t^2$, $\partial_y^2 \rightarrow d_y^2/h^2$, $\partial_x \rightarrow d_x/h$, and $\partial_t \rightarrow d_t^{c,2}/2\Delta t$, where $d_t^{c,2}f(t) = f(t + \Delta t) - f(t - \Delta t)$, the S-FD model becomes

$$\left(d_t^2 + \frac{1}{2}\frac{v\Delta t}{h}d_t^{c,2}d_x - \frac{1}{2}\frac{v^2\Delta t^2}{h^2}d_y^2\right)\psi(x, y, t)|_{x=b_x-h/2} = 0. \quad (7.89)$$

Devil in the details

The computation of $d_x\psi(b_x, y, t) = \psi(b_x + h/2, y, t) - \psi(b_x - h/2, y, t)$ requires the value of ψ at $(b_x + h/2, y)$, which lies outside of the computational

domain, so we take $x = b_x - h/2$ in Eq. (7.89); however, since $(b_x - h/2, y)$ is not a grid point, the field is unknown.

To smite this devil, we approximate the midpoint value by

$$\psi(b_x - h/2, y, t) \cong \frac{\psi(b_x - h, y, t) + \psi(b_x, y, t)}{2}. \quad (7.90)$$

Let us now discretize the computational domain by taking $t = \tau\Delta t$ and $\mathbf{x} = (x, y)h$, where $\tau = 0, 1, 2, \dots$, $x = 0, 1, \dots, x_b$, $y = 0, 1, \dots, y_b$, and $x_b h, y_b h = b_x, b_y$, respectively. Defining $\psi(\mathbf{x}, t) = \psi_{x,y}^\tau$, $d_x^2 \psi(\mathbf{x}, t) = d_x^2 \psi_{x,y}^\tau$, $d_y^2 \psi(\mathbf{x}, t) = d_y^2 \psi_{x,y}^\tau$, and $u = \nu\Delta t/h$, the S-FD model [Eq. (7.89)] becomes

$$\begin{aligned} & \left(\frac{\psi_{x_b,y}^{\tau+1} + \psi_{x_b-1,y}^{\tau+1}}{2} \right) + \left(\frac{\psi_{x_b-1,y}^{\tau-1} + \psi_{x_b,y}^{\tau-1}}{2} \right) - 2 \left(\frac{\psi_{x_b-1,y}^\tau + \psi_{x_b,y}^\tau}{2} \right) \\ & + \frac{1}{2} u \left[\left(\frac{\psi_{x_b,y}^{\tau+1} - \psi_{x_b-1,y}^{\tau+1}}{2} \right) - \left(\frac{\psi_{x_b,y}^{\tau-1} - \psi_{x_b-1,y}^{\tau-1}}{2} \right) \right] \\ & - \frac{1}{2} u^2 d_y^2 \left(\frac{\psi_{x_b,y}^\tau + \psi_{x_b-1,y}^\tau}{2} \right) = 0, \end{aligned} \quad (7.91a)$$

or

$$\begin{aligned} & (\psi_{x_b,y}^{\tau+1} + \psi_{x_b-1,y}^{\tau+1}) + (\psi_{x_b-1,y}^{\tau-1} + \psi_{x_b,y}^{\tau-1}) - 2(\psi_{x_b-1,y}^\tau + \psi_{x_b,y}^\tau) \\ & + \frac{1}{2} u \left[(\psi_{x_b,y}^{\tau+1} - \psi_{x_b-1,y}^{\tau+1}) - (\psi_{x_b,y}^{\tau-1} - \psi_{x_b-1,y}^{\tau-1}) \right] \\ & - \frac{1}{2} u^2 d_y^2 (\psi_{x_b,y}^\tau + \psi_{x_b-1,y}^\tau) = 0. \end{aligned} \quad (7.91b)$$

Solving for $\psi_{x_b,y}^{\tau+1}$, we obtain an FDTD algorithm to update the $x = b_x$ boundary:

$$\begin{aligned} \psi_{x_b,y}^{\tau+1} &= \psi_{x_b,y}^\tau + (\psi_{x_b-1,y}^\tau - \psi_{x_b-1,y}^{\tau-1}) \\ &+ \left(\frac{1-u}{1+u} \right) \left[(\psi_{x_b,y}^\tau - \psi_{x_b,y}^{\tau-1}) - (\psi_{x_b-1,y}^{\tau+1} - \psi_{x_b-1,y}^\tau) \right] \\ &+ \frac{1}{2} \left(\frac{u^2}{1+u} \right) d_y^2 (\psi_{x_b,y}^\tau + \psi_{x_b-1,y}^\tau). \end{aligned} \quad (7.92a)$$

Inside the boundary, $\psi_{x,y}^\tau$ is computed using the FDTD algorithm for the wave equation. This ABC is called the Mur⁴ absorbing boundary condition, which we henceforth call the standard (S) Mur ABC.

Devil in the details

The computation of $\psi_{x_b,y}^{\tau+1}$ requires the interior value $\psi_{x_b-1,y}^{\tau+1}$, so it must be computed first using wave equation FDTD in the interior of the computational domain.

An FDTD algorithm at the $x = 0$ boundary is obtained from Eq. (7.92a) with the substitutions $b_x \rightarrow 0$ and $b_x - h \rightarrow h$:

$$\begin{aligned} \psi_{0,y}^{\tau+1} = & \psi_{0,y}^{\tau} + (\psi_{1,y}^{\tau} - \psi_{1,y}^{\tau-1}) + \left(\frac{1-u}{1+u} \right) \left[(\psi_{0,y}^{\tau} - \psi_{0,y}^{\tau-1}) - (\psi_{1,y}^{\tau+1} - \psi_{1,y}^{\tau}) \right] \\ & + \frac{1}{2} \left(\frac{u^2}{1+u} \right) d_y^2 (\psi_{0,y}^{\tau} + \psi_{1,y}^{\tau}). \end{aligned} \quad (7.92b)$$

Defining $b=0$ on the $x = 0$ boundary, $b=x_b$ on the $x = x_b$ boundary, $i=1$ at $x = h$, and $i=b-1$ at $x = x_b - h$, the ABC expressions for the left and right boundaries can be combined into

$$\begin{aligned} \psi_{b,y}^{\tau+1} = & \psi_{b,y}^{\tau} + (\psi_{i,y}^{\tau} - \psi_{i,y}^{\tau-1}) + \left(\frac{1-u}{1+u} \right) [(\psi_{b,y}^{\tau} - \psi_{b,y}^{\tau-1}) - (\psi_{i,y}^{\tau+1} - \psi_{i,y}^{\tau})] \\ & + \frac{1}{2} \left(\frac{u^2}{1+u} \right) d_y^2 (\psi_{b,y}^{\tau} + \psi_{i,y}^{\tau}). \end{aligned} \quad (7.93a)$$

Similarly, on the $y = 0$ and $y = y_b$ boundaries, setting $b=0$ and $b=y_b$, respectively, and on the $y = h$ and $y = y_b - h$ boundaries, setting $i=1$ and $i=y_b-1$, respectively, we obtain a unified expression for the top and bottom boundaries:

$$\begin{aligned} \psi_{x,b}^{\tau+1} = & \psi_{x,b}^{\tau} + (\psi_{x,i}^{\tau} - \psi_{x,i}^{\tau-1}) + \left(\frac{1-u}{1+u} \right) [(\psi_{x,b}^{\tau} - \psi_{x,b}^{\tau-1}) - (\psi_{x,i}^{\tau+1} - \psi_{x,i}^{\tau})] \\ & + \frac{1}{2} \left(\frac{u^2}{1+u} \right) d_x^2 \left(\frac{\psi_{x,b}^{\tau} + \psi_{x,i}^{\tau}}{2} \right). \end{aligned} \quad (7.93b)$$

Devil in the details

To compute $d_y^2 \psi$ and $d_x^2 \psi$ on the corners $(x, y) = (0, 0)$, $(0, b_x)$, $(0, b_y)$, and (b_x, b_y) , we assume periodicity. For example, $d_y^2 \psi_{0,0}^{\tau} \equiv \psi_{0,1}^{\tau} + \psi_{0,y_b}^{\tau} - 2\psi_{0,0}^{\tau}$. Which one-way wave equation to apply at the corners is arbitrary. In our programs, we apply the left-right ABC first, store the corner values, then apply the top-bottom ABC and insert the stored corner values into the final output. Applying the ABC twice at the corner points can cause numerical instability.

Let us now evaluate how well the S-Mur ABC annihilates an infinite plane wave. Let us define the action of the left side of Eq. (7.89) on ψ to be $A_S\psi$, and let $\psi = e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}$, where $\mathbf{k} = k(\cos\theta, \sin\theta)$, and θ is the angle between $\mathbf{k}$ and the normal to the $x = b_x$ boundary. Because the wave is not perfectly absorbed, $A_S\psi = \varepsilon_S(\theta)\psi$, where ε_S is proportional to the reflection.

Using the identities

$$(\psi_{b_x, y}^t + \psi_{b_x - h, y}^t) = 2 \cos(k_x h/2) \psi_{b_x - h/2, y}^t, \quad (7.94a)$$

$$(\psi_{b_x, y}^t - \psi_{b_x - h, y}^t) = 2i \sin(k_x h/2) \psi_{b_x - h/2, y}^t, \quad (7.94b)$$

$$d_y^2 \psi_{x, y}^t = -4 \sin^2(k_y h/2) \psi_{x, y}^t, \quad (7.94c)$$

we find that

$$\begin{aligned} \frac{\varepsilon_S(\theta)}{8 \sin^2(\omega \Delta t/2)} &= -\cos(k_x h/2) + u \frac{\sin(k_x h/2)}{\tan(\omega \Delta t/2)} \\ &\quad + \frac{1}{2} u^2 \frac{\sin^2(k_y h/2)}{\sin^2(\omega \Delta t/2)} \cos(k_x h/2). \end{aligned} \quad (7.95)$$

Expanding $\varepsilon_S(\theta)$ in a Taylor series about $\theta = 0$, we find that

$$\begin{aligned} \frac{\varepsilon_S(\theta)}{8 \sin^2(\omega \Delta t/2)} &= \theta^0 \left[-\cos(kh/2) + u \frac{\sin(kh/2)}{\tan(\omega \Delta t/2)} \right] \\ &\quad + \frac{1}{4} \theta^2 \left[\cos(kh/2) \left(\frac{(kh)^2 u^2}{2 \sin^2(\omega \Delta t/2)} - \frac{(kh)u}{\tan(\omega \Delta t/2)} \right) \right. \\ &\quad \left. - (kh) \sin(kh/2) \right] + \cdots. \end{aligned} \quad (7.96)$$

Expanding the θ^0 term about $kh = 0$ using $\omega \Delta t = (kh)u$ yields

$$8 \sin^2(\omega \Delta t/2) \left[-\cos(kh/2) + u \frac{\sin(kh/2)}{\tan(\omega \Delta t/2)} \right] = \frac{1}{6} (kh)^4 u^2 [1 - u^2] + \cdots, \quad (7.97a)$$

and expanding the θ^2 term about $kh = 0$ yields

$$\begin{aligned} 8 \sin^2(\omega \Delta t/2) &\left\{ \cos(kh/2) \left[\frac{(kh)^2 u^2}{2 \sin^2(\omega \Delta t/2)} - \frac{(kh)u}{\tan(\omega \Delta t/2)} \right] - (kh) \sin(kh/2) \right\} \\ &= \frac{(kh)^4}{12} u^2 (2u^2 - 3) + \cdots. \end{aligned} \quad (7.97b)$$

Thus,

$$\varepsilon_S(\theta) = (kh)^4 u^2 \left[\theta^0 \frac{1}{6} (1 - u^2) + \theta^2 \frac{1}{12} (2u^2 - 3) \right] + \cdots. \quad (7.98)$$

7.5.3 Nonstandard finite difference model

We now derive a NS-FD model^{5,6} for the one-way wave equations from the S-FD model of Eq. (7.89). Setting $\nu\Delta t/h \rightarrow u$, Eq. (7.89) becomes

$$\left(d_t^2 + \frac{1}{2}ud_t^{c,2}d_x - \frac{1}{2}u^2d_y^2\right)\psi(x, y, t)|_{x=b_x-h/2} = 0. \quad (7.99)$$

We now treat u and u^2 as free, independent parameters that we can choose to minimize the reflection. Putting $u \rightarrow \tilde{v}_1$ and $u^2 \rightarrow \tilde{v}_2^2$, we obtain the NS model

$$\left(d_t^2 + \frac{1}{2}\tilde{v}_1d_t^{c,2}d_x + \frac{1}{2}\frac{\tilde{v}_2^2\Delta t^2}{h^2}d_y^2\right)\psi(x, y, t)|_{x=b_x-h/2} = 0. \quad (7.100)$$

Following the derivation of $\varepsilon_S(\theta)$ given by Eq. (7.95), we find the error of the NS model to be

$$\begin{aligned} \frac{\varepsilon_{NS}(\theta)}{8\sin^2(\omega\Delta t/2)} &= -\cos(k_x h/2) + \tilde{v}_1 \frac{\sin(k_x h/2)}{\tan(\omega\Delta t/2)} \\ &\quad + \frac{1}{2}\tilde{v}_2^2 \frac{\sin^2(k_y h/2)}{\sin^2(\omega\Delta t/2)} \cos(k_x h/2). \end{aligned} \quad (7.101)$$

We now proceed to minimize the error. To simplify the algebra, we write

$$\tilde{v}_1 = w_1 \tan(\omega\Delta t/2), \quad (7.102a)$$

$$\tilde{v}_2^2 = w_2^2 \sin^2(\omega\Delta t/2), \quad (7.102b)$$

$$\begin{aligned} \frac{\varepsilon_{NS}(\theta)}{8\sin^2(\omega\Delta t/2)} &= -\cos(k_x h/2) + w_1 \sin(k_x h/2) \\ &\quad + \frac{1}{2}w_2^2 \sin^2(k_y h/2) \cos(k_x h/2). \end{aligned} \quad (7.103)$$

We are now free to adjust w_1 and w_2 to minimize the error at two desired incidence angles. For a general-purpose ABC, let us require that $\varepsilon_{NS}(0) = 0$. At $\theta = 0$, $k_x = k$, and $k_y = 0$; thus,

$$w_1 = \cot(kh/2) \quad (7.104)$$

gives $\varepsilon_{NS}(0) = 0$. Next, requiring that $\varepsilon_{NS}(\theta_2) = 0$ gives

$$w_2^2 = 2 \left[\frac{\tan(kh/2) - \tan(kh \cos \theta_2/2)}{\tan(kh/2) \sin^2(kh \sin \theta_2/2)} \right]. \quad (7.105a)$$

The larger θ_2 the greater the absorption at high incidence angles, but the greater the reflection at intermediate angles, $0 < \theta \leq \theta_2$. We have examined

various choices for θ_2 and conclude that the best overall choice is $\theta_2 = \pi/4$. When waves are incident over a wide range of large angles, however, $\theta_2 = \pi/3$ is also a reasonable compromise. For specialty applications, one could also require that $\varepsilon_{\text{NS}}(\theta_1) = \varepsilon_{\text{NS}}(\theta_2) = 0$. Henceforth, unless otherwise specified, $\theta_2 = \pi/4$, and

$$w_2^2 = 2 \left[\frac{\tan(kh/2) - \tan(kh\sqrt{2}/4)}{\tan(kh/2) \sin^2(kh \sin \sqrt{2}/4)} \right]. \quad (7.105b)$$

From Eq. (7.102a) we now have

$$\tilde{v}_1 = \frac{\tan(\omega\Delta t/2)}{\tan(kh/2)}, \quad (7.106a)$$

$$\tilde{v}_2^2 = 2 \sin^2(\omega\Delta t/2) \left[\frac{\tan(kh/2) - \tan(kh \cos \theta_2/2)}{\tan(kh/2) \sin^2(kh \sin \theta_2/2)} \right]. \quad (7.106b)$$

On the $x = 0$ and $x = x_b$ boundaries, the NS version of the Mur ABC now becomes

$$\begin{aligned} \psi_{b,y}^{\tau+1} = & \psi_{b,y}^{\tau} + (\psi_{i,y}^{\tau} - \psi_{i,y}^{\tau-1}) + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) [(\psi_{b,y}^{\tau} - \psi_{b,y}^{\tau-1}) - (\psi_{i,y}^{\tau+1} - \psi_{i,y}^{\tau})], \\ & + \frac{1}{2} \left(\frac{\tilde{v}_2^2}{1 + \tilde{v}_1} \right) d_y^2 (\psi_{b,y}^{\tau} + \psi_{i,y}^{\tau}), \end{aligned} \quad (7.107a)$$

and on the $y = 0$ and $y = x_b$ boundaries,

$$\begin{aligned} \psi_{x,b}^{\tau+1} = & \psi_{x,b}^{\tau} + (\psi_{x,i}^{\tau} - \psi_{x,i}^{\tau-1}) + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) [(\psi_{x,b}^{\tau} - \psi_{x,b}^{\tau-1}) - (\psi_{x,i}^{\tau+1} - \psi_{x,i}^{\tau})] \\ & + \frac{1}{2} \left(\frac{\tilde{v}_2^2}{1 + \tilde{v}_1} \right) d_x^2 \left(\frac{\psi_{x,b}^{\tau} + \psi_{x,i}^{\tau}}{2} \right). \end{aligned} \quad (7.107b)$$

We call Eq. (7.107) the NS-Mur ABC.

Both the S-Mur and NS-Mur ABCs can be straightforwardly extended to three dimensions.

7.5.4 Numerical stability of the Mur absorbing boundary condition

S-Mur ABC

The stability of the S- and NS-Mur ABCs is analyzed in Appendix 7.2. For the S-Mur ABC, we can analytically obtain the 2D and 3D stability conditions. We have confirmed the following practical stability limits:

$$\frac{v\Delta t}{h} \leq 0.67 \quad \text{in two dimensions,} \quad (7.108a)$$

$$\frac{v\Delta t}{h} \leq 0.45 \quad \text{in three dimensions.} \quad (7.108b)$$

The 2D limit is slightly less than the analytically derived stability limit (0.70) for the S-FDTD algorithm, and in three dimensions is somewhat lower than the analytical stability limit (0.57) for S-FDTD.

NS-Mur ABC

The stability analysis of the NS-Mur ABC is much more difficult because $\tilde{v}_1$ and $\tilde{v}_2^2$ have a complicated relationship. We have, however, numerically verified that the NS-Mur ABC is stable when $\tilde{v}_1$ and $\tilde{v}_2^2$ are given by Eq. (7.102) in both two and three dimensions.

As shown in Eq. (A7.2), the stability conditions are $\tilde{v}_1 < 4$ (true for all practical algorithms in both two and three dimensions) and

$$\tilde{v}_2^4 + \tilde{v}_2^2 \tilde{v}_1 - 2\tilde{v}_2^2 + \frac{1}{4}\tilde{v}_1^2 - \tilde{v}_1 \leq 0, \quad \text{in two dimensions,} \quad (7.109a)$$

$$4\tilde{v}_2^4 + 2\tilde{v}_2^2 \tilde{v}_1 - 4\tilde{v}_2^2 + \frac{1}{4}\tilde{v}_1^2 - \tilde{v}_1 \leq 0, \quad \text{in three dimensions.} \quad (7.109b)$$

These conditions are satisfied by all practical algorithms, where $\tilde{v}$ is within the stability limits of Eq. (7.23).

7.5.5 Comparison of S- and NS-Mur ABCs

Using a modification of the test described in Refs. 7 and 8, we evaluate the performance of the NS-Mur ABC. We generalize the pulse defined by Eq. (6.46) (p. 258 of Ref. 8) to

$$p_0(t) = \frac{1}{32} [10 - 15 \cos(0.5\omega_m t) + 6 \cos(\omega_m t) - \cos(1.5\omega_m t)] \quad \text{for } 0 \leq t \leq 2T_m, \\ = 0 \quad \text{for } t > T_m, \quad (7.110)$$

where $T_m = 2\pi/\omega_m$. We use p_0 to modulate a sinusoidal source of angular frequency ω using $T_m = 16T$, where $T = 2\pi/\omega$. The point source, $s(t) = p_0(t) \sin(\omega t)$, is positioned in the center of a $6\lambda \times 3\lambda$ computational domain, where λ is the wavelength corresponding to ω . We take $\lambda = 8h$, and following Ref. 8, set $v\Delta t/h = 0.5$ so that $T = 16\Delta t$. Using S-FDTD with the S-Mur ABC and NS-FDTD with the NS-Mur ABC, we evaluate the mean global energy, $E(t) = (1/N) \sum_{x,y} |\psi(x, y, t)|^2$, as a function of time step, where N is the number of grid points. The result is shown in Fig. 7.2.

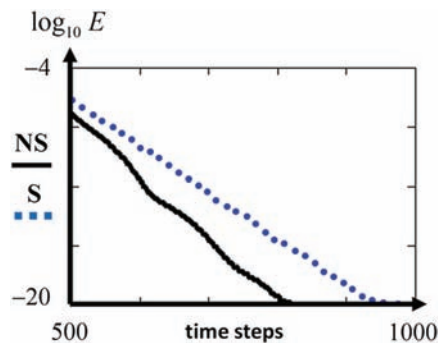


Figure 7.2 The S-Mur ABC versus the NS-Mur ABC. Energy fall-off is due to a pulse-modulated sine source in the center of a $6\lambda \times 3\lambda$ computational domain, $\lambda = 8h$, $\nu\Delta t/h = 0.5$; the source turns off at $t = 512\Delta t$.

Obviously, the NS-Mur ABC gives superior absorption. After 800 time steps, the energy for the NS-Mur ABC is 10^{-4} times that for the S-Mur ABC.

Next, we evaluate the reflected intensity as a function of incidence angle on the computational boundary, as shown in Fig. 7.3. Replacing $\omega_m t$ with $k_m(x + \lambda_m)$ and T_m with λ_m in Eq. (7.110) gives a spatial modulation function centered about $x = 0$:

$$p_0(x) = \frac{1}{32} \{ 10 - 15 \cos[0.5k_m(x + \lambda_m)] + 6 \cos[k_m(x + \lambda_m)] - \cos[1.5k_m(x + \lambda_m)] \} \times \Theta(\lambda_p - |x|), \quad (7.111)$$

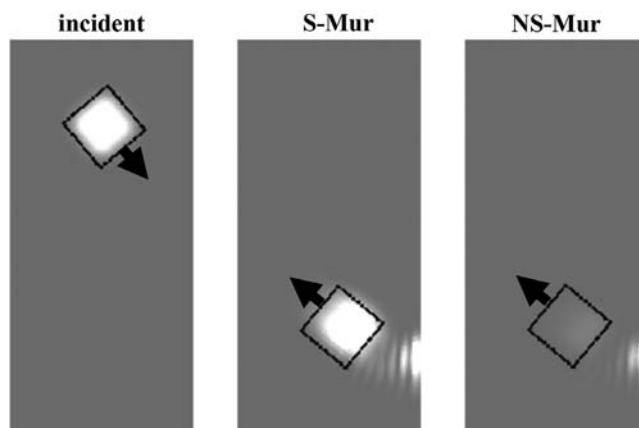


Figure 7.3 A pulse propagated onto the right computational boundary at an angle $\theta_i = 50$ deg, where either the S-Mur ABC or the NS-Mur ABC is enforced. Notice that reflection angle $\theta_r \neq \theta_i$.

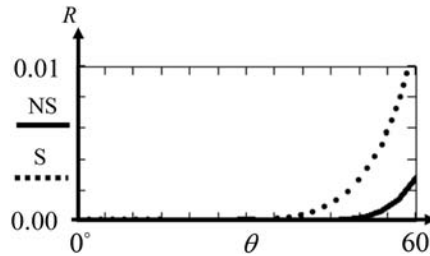


Figure 7.4 Intensity reflection coefficient R versus incidence angle θ for the S- and NS-Mur ABCs. Up to about $\theta = 60$ deg, the NS-Mur ABC gives low reflection, after which it rises rapidly.

where θ is the step function. We use Eq. (7.111) to spatially modulate an incident plane wave of wavelength $\lambda = 2\pi/k$. This gives the incident waveform of Fig. 7.3 with $\lambda_m = 3\lambda$, which implies that $k_m = k/3$.

Using NS-FDTD ($\lambda = 8h$, $\tilde{\nu} = 0.80$) with the NS-Mur ABC, and S-FDTD ($\lambda = 8h$, $\nu\Delta t/h = 0.68$) with the S-Mur ABC, we propagate the pulse onto the right boundary at various incidence angles θ_i to obtain the reflection spectrum of the S- and NS-Mur ABCs. The pulse position (square outline in Fig. 7.3) is computed under the assumption that the angle of reflection θ_r equals the angle of incidence and that pulse group velocity equals phase velocity; however, as the figure shows, $\theta_r \neq \theta_i$, and the reflected pulse is not exactly centered within the box; also, some energy remains on the boundary. The incident intensity I_i and the reflected intensity I_r are the mean intensities of the pulse within the box, and the intensity reflection coefficient is $R = I_r/I_i$. The reflection spectra are shown in Fig. 7.4. A computational implementation of the S- and NS-Mur ABCs is given in Program MC7.1.

The NS-Mur ABC is low cost and easy to implement; it requires just two grid points (the boundary and the first interior point). When better performance is required, the best ABC currently available is the “perfectly matched layer” (PML). Although the PML is more complicated and costly to implement, it can be made—in principle (with some limitations)—arbitrarily close to a perfect ABC. We omit this topic because it would take many pages to properly develop it and to exorcise all of the devils in the details. The PML methodology is derived and its implementation explained in Refs. 9 and 10. Methodologies based on discrete Green’s functions have also been proposed to terminate the computational boundary.^{11–14}

7.6 Object Models on the Grid

Before proceeding to solve interesting problems, we must develop models of objects on the grid. In one dimension, we can take the size of a simple object to be an integer number of grid spacings; however, in two dimensions, even if the radius of a circle (for example) is an integer number of grid units along the

principal axes, in other directions its boundary runs between the grid points. Thus, we must model material boundaries that lie between the grid points. For this purpose, we now develop what we call the “fuzzy” model.

7.6.1 Model of a dielectric

In one dimension, let the scatterer S be a uniform layer of width w and the refractive index n_s be relative to the medium in which it is immersed. It is convenient to introduce an “inclusion” function $S(x)$ defined by

$$\begin{aligned} S(x) &= 1 \quad \text{for } x \in S \\ S(x) &= 0 \quad \text{for } x \notin S, \end{aligned} \quad (7.112)$$

where S is the set of grid points inside the scatterer. This grid representation is often called the “staircase” model (the reason will become evident in two and three dimensions). The index of refraction is a function of position given by $n(x) = n_s$ for $x \in S$, and $n(x) = 1$ for $x \notin S$. Thus,

$$n(x) = 1 + (n_s - 1)S(x). \quad (7.113)$$

Expressing the 1D wave equation in the form

$$n(x)^2 \partial_t^2 \psi(x, t) = v_0^2 \partial_x^2 \psi(x, t), \quad (7.114)$$

let $g = m\Delta x$ (m is an integer) be a grid point within the computational domain. Spatially integrating over $g - \Delta x/2 \leq x \leq g + \Delta x/2$ gives

$$\partial_t^2 \int_{g-\frac{\Delta x}{2}}^{g+\frac{\Delta x}{2}} n(x)^2 \psi(x, t) dx = v_0^2 \int_{g-\frac{\Delta x}{2}}^{g+\frac{\Delta x}{2}} \partial_x^2 \psi(x, t) dx. \quad (7.115)$$

If both the incident wavelength λ_0 and λ_0/n_s are large compared to Δx , then $\psi(x, t)$ changes slowly over the integration interval and can be taken outside of the integration on both sides of Eq. (7.115) to give

$$\Delta x \langle n(g)^2 \rangle \partial_t^2 \psi(g, t) = v_0^2 \Delta x \partial_x^2 \psi(x, t)|_{x=g}, \quad (7.116)$$

where

$$\langle n(g)^2 \rangle = \frac{1}{\Delta x} \int_{g-\frac{\Delta x}{2}}^{g+\frac{\Delta x}{2}} n(x)^2 dx \quad (7.117)$$

is the average value of n^2 about g . Using the fact that $S(x)^2 = S(x)$, we can express $\overline{n(g)^2}$ in terms of the averaged or fuzzy inclusion function defined by

$$\bar{S}(g) = \frac{1}{\Delta x} \int_{g-\frac{\Delta x}{2}}^{g+\frac{\Delta x}{2}} dx S(x). \quad (7.118)$$

While S takes the binary values 0 and 1, $0 \leq \bar{S} \leq 1$ is a fuzzy logical function. In terms of $\bar{S}$,

$$\langle n(x)^2 \rangle = 1 + (n_s^2 - 1)\bar{S}(g), \quad (7.119)$$

which is useful for computational purposes. Thus, at grid point g , the wave equation becomes

$$\left[\partial_t^2 - \frac{v_0^2}{\langle n(x)^2 \rangle} \right] \partial_x^2 \psi(x, t)|_{x=g} = 0. \quad (7.120)$$

This model is not exact, but it is much better than the staircase model. A practical implementation of the fuzzy model is given in Program MCL.1.

Devil in the details

For arbitrary shapes, a subgrid is used to compute $\bar{S}(g)$, but the error of the model does not necessarily decrease monotonically with subgrid size, especially for a small number of subgrids.

7.6.2 Model of an absorbing dielectric

Let the absorption be given by $\alpha(x) = \alpha_s$ for $x \in \mathbf{S}$, and $\alpha(x) = 0$ for $x \notin \mathbf{S}$. Thus,

$$\alpha(x) = \alpha_s S(x). \quad (7.121)$$

Expressing the absorbing wave equation in the form

$$[n(x)^2 \partial_t^2 + 2\alpha(x) \partial_t] \psi(x, t) = v_0^2 \partial_x^2 \psi(x, t) \quad (7.122)$$

and following the procedure of the previous section, it is easy to see that

$$\begin{aligned} \langle \alpha(g) \rangle &= \frac{1}{\Delta x} \int_{g-\frac{\Delta x}{2}}^{g+\frac{\Delta x}{2}} \alpha(x) dx \\ &= \alpha_s \bar{S}(g). \end{aligned} \quad (7.123)$$

Thus, at grid point g , the absorbing wave equation becomes

$$\left[\partial_t^2 + 2\langle \alpha(x) \rangle - \frac{v_0^2}{\langle n(x)^2 \rangle} \right] \partial_x^2 \psi(x, t)|_{x=g} = 0. \quad (7.124)$$

7.6.3 Generalization to two and three dimensions

To generalize the averaging process to $d =$ two or three dimensions, we simply replace the linear integrals by area and volume integrals. Thus,

$$\bar{S}(\mathbf{g}) = \frac{1}{h^d} \int_{V(\mathbf{g})} d^d \mathbf{x} S(\mathbf{x}), \quad (7.125)$$

where $\mathbf{g} = (g_x, g_y)$, $\mathbf{x} = (x, y)$, and $d^2 \mathbf{x} = dxdy$ in two dimensions, and $\mathbf{g} = (g_x, g_y, g_z)$, $\mathbf{x} = (x, y, z)$, and $d^3 \mathbf{x} = dxdydz$ in three dimensions. The integration region is

$$\begin{aligned} V(\mathbf{g}) &= (g_x - h/2 \leq x \leq g_x + h/2) \times (g_y - h/2 \leq y \leq g_y + h/2), \\ V(\mathbf{g}) &= (g_x - h/2 \leq x \leq g_x + h/2) \times (g_y - h/2 \leq y \leq g_y + h/2) \\ &\quad \times (g_z - h/2 \leq z \leq g_z + h/2) \end{aligned}$$

in two and three dimensions, respectively.

Figure 7.5 depicts the representation of a solid circle in the staircase (top) and fuzzy models (bottom) for different positions of the circle center on the grid. While the geometric shape changes with shifts in the center position in both models, the fuzzy model preserves the area.

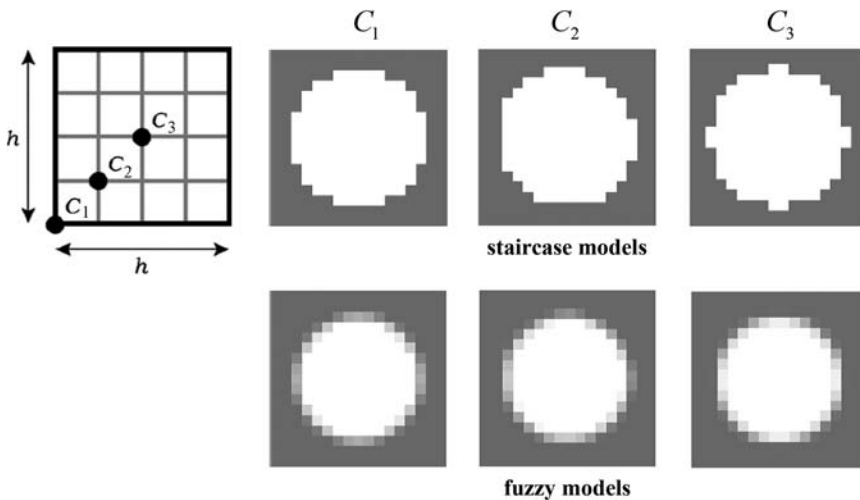


Figure 7.5 Visualization of the inclusion function for the staircase (top) and fuzzy models (bottom) of a solid circle for different positions of its center. C_1 is on the grid line, and C_3 is centered in the $h \times h$ pixel; C_2 is midway between C_1 and C_3 . White corresponds to 100% inclusion, and gray corresponds to 0% inclusion.

In two and three dimensions, we now have

$$\langle n^2(\mathbf{g}) \rangle = 1 + (n_s^2 - 1)\bar{S}(\mathbf{g}), \quad (7.126)$$

$$\langle \alpha(\mathbf{g}) \rangle = \alpha_s \bar{S}(\mathbf{g}). \quad (7.127)$$

7.6.4 Numerical examples

Let S be a small circle of radius $r = 1.2h$ on a 2D grid. In the staircase model $[S(\mathbf{x}) = 0 \text{ or } 1]$, as shown in Fig. 7.6, the representation depends on the location of the circle center c . Not only does the geometric shape change with shifts of c , but the area $A = \sum_{\mathbf{x} \in S} S(\mathbf{x})$ also changes. For $c = (2, 2)h$, $A = 5h^2$, while for $c = (3/2, 5/2)h$, $A = 4h^2$; obviously, $A \neq \pi r^2$. On the other hand, in the fuzzy representation ($0 \leq \bar{S} \leq 1$), as shown in Fig. 7.7, the geometric shape does vary with shifts in c , but $A = \pi r^2$ is invariant.

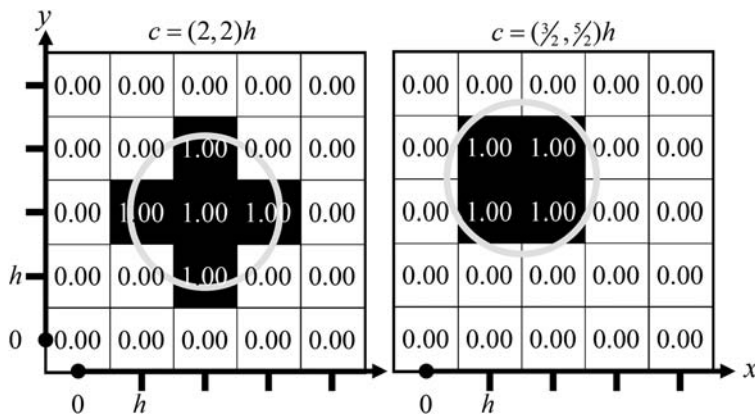


Figure 7.6 Staircase model. Grid representation of a circle of radius $r = 1.2h$ centered at c . The center of each pixel is a grid point. Numbers indicate the value of S at the pixel center.

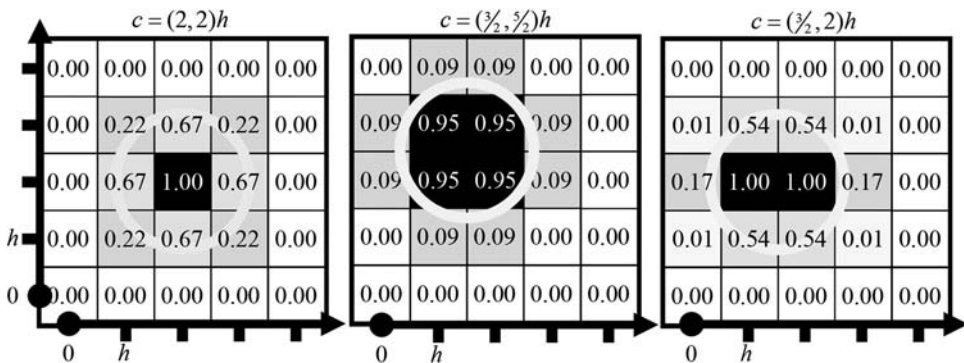


Figure 7.7 Fuzzy model. Grid representation of a circle of radius $r = 1.2h$ centered at c . The center of each pixel is a grid point. Numbers indicate the value of S at the pixel center.

7.7 Mie Scattering and Validation of Computations

We are now ready to combine the results of the previous sections to do interesting calculations. First, let us confirm that our methodology is correct by comparing computations with analytical solutions. For this purpose, we choose Mie scattering. In the Mie regime, the incident wavelength λ_0 is on the same order of magnitude as the size s of the scatterer ($\lambda_0 \sim s$). The full form of the wave equation, without simplification, must be solved subject to the boundary conditions. Analytic solutions exist for only a few highly symmetric objects, such as spheres and infinite cylinders. It is a challenge for any numerical algorithm to accurately compute Mie scattering; therefore, analytic solutions of Mie scattering can be used to validate numerical algorithms, such as FDTD. Formulae to compute a few analytic solutions are given in Appendices 10.1 and 10.2.

Using S- and NS-FDTD, we computed the scattered field ψ_s due to a 2D infinite plane wave incident from vacuum on a circular region of refractive index n_s . This configuration is equivalent to the 3D case of an infinite plane wave incident perpendicularly to the axis of an infinite cylinder. This is because the fields and physical parameters are all invariant with respect to translation along the cylinder axis. Looking ahead to Chapter 10, we will see that an infinite plane scalar wave scattering off the cylinder is equivalent to an infinite plane electromagnetic wave scattering off the cylinder in the TE mode (electric-field polarized parallel to the cylinder axis).

For the calculation depicted in Fig. 7.8, we use a cylinder of radius $a = 0.75\lambda_0$ centered on the z axis with $n_s = 1.7$. In the FDTD calculations, we take $h = \lambda_0/8$ (inside the cylinder $h = n_s\lambda_0/8 \cong 4.7$). The computed scattered intensity $|\psi_s|^2$ is visualized outside the cylinder in shades of red and compared with the analytic solution given by Mie theory.

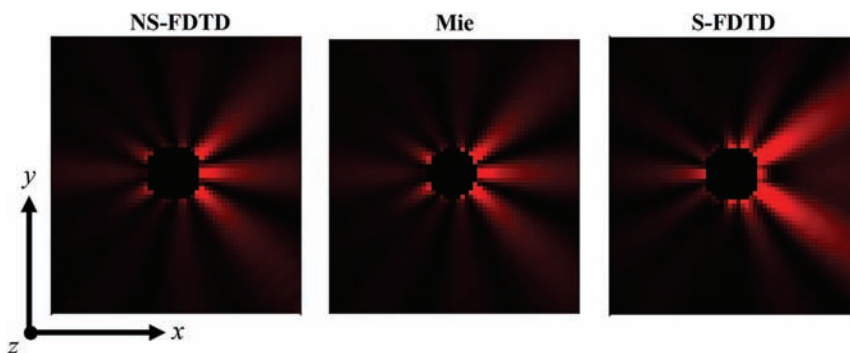


Figure 7.8 Scattered intensity due to a plane wave incident on a dielectric cylinder. Intensity is visualized in shades of red; black = zero field or cylinder interior. The incident field is along the x axis.

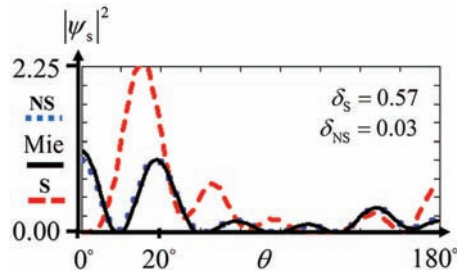


Figure 7.9 Scattered intensity on a contour of radius $1.25\lambda_0$ about the disk center as a function of angle θ from the incident direction; δ denotes root-mean-square deviation from Mie theory.

In Fig. 7.9, $|\psi_s|^2$ is plotted on a circular contour of radius $1.25\lambda_0$ about the cylinder center as a function scattering angle from the incident direction. Obviously, NS-FDTD gives superior accuracy. Program MC7.2 is an implementation of the scattered-field calculation in two dimensions.

7.7.1 Effect of grid representation

The total error of an FDTD calculation is due not only to algorithm error, but also to grid representation error and errors due to the termination of the computational domain. Since the error of NS-FDTD is very low, the grid representation error dominates.

Let us replace the large cylinder of Figs. 7.8 and 7.9 with a slender cylinder centered at different positions on the grid. We take its refractive index to be $n_s = 1.5$ and the incident wavelength to be $\lambda_0/h = 8$, radius $r = 1.2h$, which implies that $r = 0.15\lambda_0$. Figure 7.10 compares the scattered intensity computed using NS-FDTD with the fuzzy model to Mie theory for different

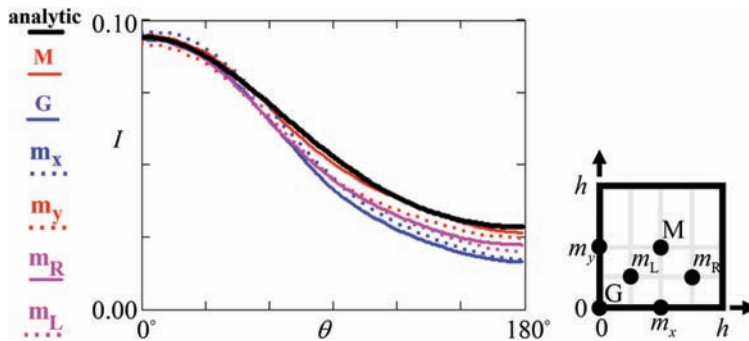


Figure 7.10 Effect of grid representation on the NS-FDTD calculation of the angular distribution of scattered intensity $I(\theta)$. Cylinder radius $= r = 1.2h$, and $I(\theta)$ is evaluated on a contour of radius $5r$ about the cylinder center. The NS-FDTD results for different cylinder centers are compared with the analytic result given by Mie theory. The incident wavelength discretization is $\lambda_0/h = 8$.

positions of the cylinder center. Position M is the center of an $h \times h$ pixel, while G is exactly on a grid point; other centers are located as shown.

We see that when the cylinder is centered in the middle of a grid pixel (position M), the accuracy is highest. If the purpose were simply to compute the scattering off of just one cylinder, it could always be optimally centered, but often we want to compute transmission through or reflection off an array, such as a photonic crystal, for which it is impossible to optimally center each cylinder.

Fortunately, when the incident wavelength is large compared to the cylinder radius, the errors over the whole array are small enough to allow calculation of the bandgap with reasonable accuracy.

7.8 Discrete Green's Function Solution of the Scattering Problem

7.8.1 Discrete Green's functions

We can straightforwardly extend the discrete Green's function (DGF) methodology of Section 6.6 to two and three dimensions.

The 2D DGF in free space g is the solution of

$$\left(d_\tau^2 - \tilde{v}_0^2 \tilde{\mathbf{d}}^2\right) g_{\mathbf{x}-\mathbf{x}'}^{\tau-\tau'} = \delta_{\mathbf{x}-\mathbf{x}',0} \delta_{\tau-\tau',0} \quad (7.128)$$

for NS-FDTD; for S-FDTD it is the solution of

$$\left(d_\tau^2 - u_0^2 \mathbf{d}^2\right) g_{\mathbf{x}-\mathbf{x}'}^{\tau-\tau'} = \delta_{\mathbf{x}-\mathbf{x}',0} \delta_{\tau-\tau',0}, \quad (7.129)$$

where $\mathbf{x} = (x, y)h$, and $t = \tau\Delta t$. For NS-FDTD, we take $\tilde{v}_0 = 0.80$ and make the substitution $\tilde{\mathbf{d}}^2 \rightarrow \mathbf{d}_{1/6}^2 = \mathbf{d}^2 + (1/6) d_x^2 d_y^2$, which is frequency independent; for S-FDTD, we take $u_0 = 0.70$. Taking, $\mathbf{x}' = (0, 0) \equiv \mathbf{0}$, $\tau' = 0$, and the initial conditions $g_x^{-1} = g_x^0 = 0$, we compute the DGFs shown in Fig. 7.11.

Because the grid speed limits are different in each case (see Appendix 7.1), the NS-DGF and S-DGF cannot be exactly compared, but it is obvious from Fig. 7.11 that the NS-DGF is more symmetric. This is even more evident in Fig. 7.12, where the visualization has been adjusted to show the very low-amplitude precursor field. The S-FDTD precursor field is fundamentally square, while the NS-FDTD precursor field is circular.

In Fig. 7.13, a cross-section of g_x^{34} along the x axis is plotted and compared with the 2D free-space Green's function G given by Eq. (7.34) with $\mathbf{x}' = (0, 0)$, $\mathbf{x} = (x, 0)$, $t' = 0$, and $t = 34\Delta t$, using $v = \tilde{v}_0 = 0.83$. While G diverges when $v^2(t - t') = |\mathbf{x} - \mathbf{x}'|^2$, g is always finite.

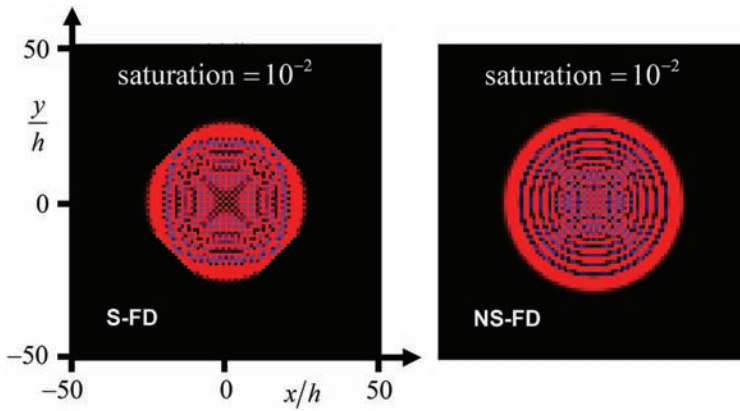


Figure 7.11 Discrete Green's functions after 34 time steps g_x^{34} calculated using S-FDTD and NS-FDTD. Values are visualized in shades of red (positive) and blue (negative). The deepest shade corresponds to $|g_x^{34}| \geq +10^{-2}$.

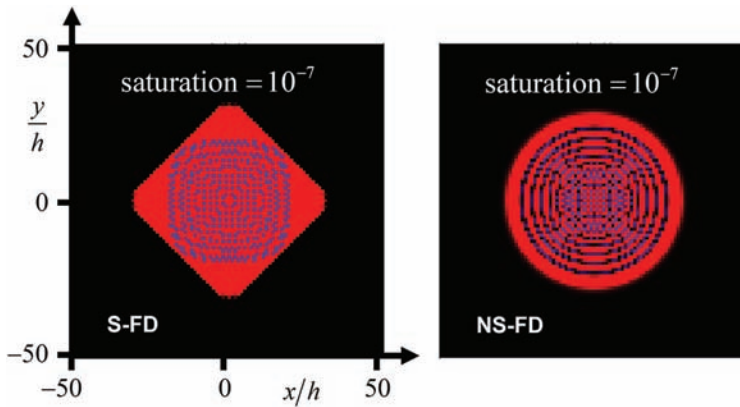


Figure 7.12 Discrete Green's functions after 34 time steps g_x^{34} calculated using S-FDTD and NS-FDTD. Values are visualized in shades of red (positive) and blue (negative). The deepest shade corresponds to $|g_x^{34}| \geq +10^{-7}$.

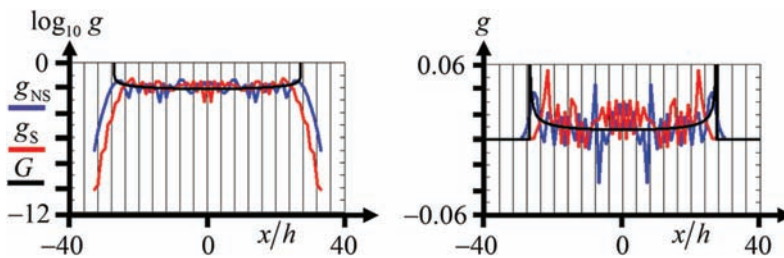


Figure 7.13 Analytic Green's function $G(\mathbf{x}, 34\Delta t)$ compared with g_x^{34} computed using S-FDTD (g_s) and NS-FDTD (g_{NS}) in free space.

7.8.2 Applications of discrete Green's functions

Let η be the size of a feature, such as the depth of a groove of a subwavelength diffraction grating, h be the grid spacing, and λ the wavelength. To represent the groove on the grid, we must choose $h/\eta \leq 1$. Thus, if $\eta \gg \lambda$, then λ/h is large, and so is the computational cost, which scales as $(\lambda/h)^4$. As we have seen, the error of the FDTD algorithm is a function of h/λ , but for $h/\eta \gg h/\lambda$, the total calculation error is dominated by grid representation error, which is a function of h/η .

It is thus desirable to have a methodology to compute the long-wavelength scattering using a smaller value of h/η (perhaps 1/2 or less) for low values of λ/h , where NS-FDTD delivers high accuracy with low computational cost.

The DGF methodology offers a reasonable solution, especially when one needs to compute a spectrum. We take the NS-FD model of the scattered-field wave equation to be

$$\left(d_\tau^2 - \frac{\tilde{v}_0^2}{\tilde{n}_x^2} \tilde{\mathbf{d}}^2\right) \psi_s|_{\mathbf{x}}^\tau = \tilde{s}_x^\tau, \quad (7.130)$$

where $\tilde{s}_x^\tau$ is the NS model of the source of the scattered field. Assuming that all of the sources turn on simultaneously at $t = 0$, the DGF to solve Eq. (7.128) satisfies

$$\left(d_\tau^2 - \frac{\tilde{v}_0^2}{\tilde{n}_x^2} \tilde{\mathbf{d}}^2\right) g_{\mathbf{x}-\mathbf{x}'}^\tau = \delta_{\mathbf{x}-\mathbf{x}',0} \delta_{\tau,0}. \quad (7.131)$$

Given g , the solution of Eq. (7.130) is

$$\psi_s|_{\mathbf{x}}^\tau = \sum_{\tau'=0}^{\tau} \sum_{\mathbf{x}' \in S} \tilde{s}_{\mathbf{x}'}^{\tau'} g_{\mathbf{x}-\mathbf{x}'}^{\tau-\tau'}, \quad (7.132)$$

where the summation is over all grid points within the scatterer S outside of which g vanishes.

As explained in Note 7.2, it is often an excellent approximation to take $\tilde{\mathbf{d}}^2 = \tilde{\mathbf{d}}^2(k_0)$; alternatively, we can put $\tilde{\mathbf{d}}^2 \rightarrow \mathbf{d}_{1/6}^2$, as was done in the computation of the free-space DGF. Outside the scatterer, $\tilde{v}_0$ is assigned the largest value consistent with algorithm stability. If the refractive index of the scatterer is greater than 1, then $\tilde{v}_0 = \sqrt{3}/2$ in two dimensions, and $\tilde{v}_0 = \sqrt{15/23}$ in three.

Suppose that we wish to compute the spectrum over the angular frequency band $\omega_1 \leq \omega \leq \omega_2$. If the band is relatively narrow, we can take $\tilde{n}$ to be its value in the middle of the band; otherwise, we can run two calculations, one with $\tilde{n}(\omega_1)$ and another with $\tilde{n}(\omega_2)$, and interpolate the DGF following the method described in Section 6.5.4.

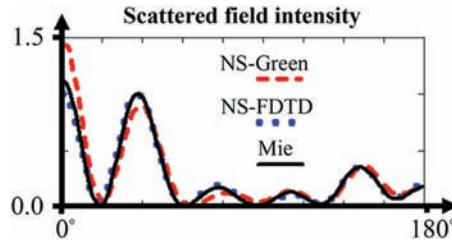


Figure 7.14 Comparison of the NS-FDTD and the DGF solutions.

Taking the initial conditions to be $g_{\mathbf{x}-\mathbf{x}'}^{-1} = g_{\mathbf{x}-\mathbf{x}'}^0 = 0$, we replace $\tau - \tau'$ by $\bar{\tau}(\tau - \tau' \rightarrow \bar{\tau})$. The DGF can now be computed using FDTD:

$$g_{\mathbf{x}-\mathbf{x}'}^{\bar{\tau}+1} = -g_{\mathbf{x}-\mathbf{x}'}^{\bar{\tau}-1} + \left(2 + \frac{\tilde{v}_0^2}{\tilde{n}_x^2} \tilde{\mathbf{d}}^2\right) g_{\mathbf{x}-\mathbf{x}'}^{\bar{\tau}} + \Delta_{\mathbf{x},\mathbf{x}'} \Delta_{\bar{\tau},0}. \quad (7.133)$$

For the scattering problem of Figs. 7.8 and 7.9, we computed the scattered field using NS-FDTD and the DGF given by Eq. (7.131), and computed using NS-FDTD. In Fig. 7.14, we compare the NS-FDTD and the DGF solution (labeled NS-Green) with the analytic solution given by Mie theory. Although NS-Green is not as accurate as NS-FDTD, it is still far more accurate than S-FDTD. For a spectrum calculation, once g is known, any source can be used.

When $\eta \ll \lambda$ is large, we can choose wavelength $\lambda_\eta \sim \eta$ to compute g and then put in a source with wavelength $\eta \ll \lambda$ to compute the optical properties. Thus, the DGF method is useful for computing spectra and can be used to reduce the computational cost when the scattering object has features small compared to the wavelength.

This methodology has been extended to Maxwell's equations.

Important Topics of Chapter 7

- S- and NS-FDTD in two and three dimensions
- Practical FDTD stability constraints; grid speed limit higher in NS-FDTD
- Broadband NS-FDTD
- The fuzzy representation of structures on the grid
- The Mur absorbing boundary condition and its NS version
- Validation of NS-FDTD for Mie scattering
- Discrete Green's function methodology

Appendix 7.1 Stability Analysis of the FDTD Algorithm for the Wave Equation

A7.1.1 Standard FDTD

The wave equation

$$(\partial_t^2 - v^2 \nabla^2) \psi(\mathbf{x}, t) = 0 \quad (\text{A7.1.1})$$

can be modeled by a finite difference equation of the form

$$(d_t^2 - u^2 \mathbf{d}^2)\psi(\mathbf{x}, t) = 0, \quad (\text{A7.1.2})$$

where $\mathbf{d}^2 = d_x^2 + d_y^2 + d_z^2$, and d_t^2 are defined in Chapter 1. In the standard finite difference (S-FD) model, $u = \nu \Delta t/h$, where $h = \Delta x = \Delta y = \Delta z$.

Expanding $d_t^2\psi(\mathbf{x}, t)$, we obtain

$$\psi(\mathbf{x}, t + \Delta t) + \psi(\mathbf{x}, t - \Delta t) - (2 + u^2 \mathbf{d}^2)\psi(\mathbf{x}, t) = 0. \quad (\text{A7.1.3})$$

Now we take $\psi = \varphi_{\mathbf{k}}$, where $\varphi_{\mathbf{k}}(\mathbf{x}, t) = e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}$ is an infinite plane wave, $\mathbf{k} = (k_x, k_y, k_z)$ is a wave vector of magnitude $k = |\mathbf{k}|$, and $\omega = \nu k$. Any monochromatic solution can be expressed as a Fourier sum in the form

$$\psi(\mathbf{x}, t) = \sum_{\mathbf{k}} c_{\mathbf{k}} \varphi_{\mathbf{k}}(\mathbf{x}, t), \quad (\text{A7.1.4})$$

where the sum is over all possible wave vector directions (of the same magnitude), and the $c_{\mathbf{k}}$ are constants. We can therefore analyze the numerical stability of the FDTD algorithm with respect to an arbitrary Fourier component. Using

$$d_x^2 e^{ik_x x} = -2[1 - \cos(kh)]e^{ik_x x}, \quad (\text{A7.1.5})$$

we find that

$$\mathbf{d}^2 \varphi_{\mathbf{k}} = -2D \varphi_{\mathbf{k}}, \quad (\text{A7.1.6})$$

where

$$D = [1 - \cos(k_x h)] + [1 - \cos(k_y h)] + [1 - \cos(k_z h)]. \quad (\text{A7.1.7})$$

Thus, Eq. (A7.1.3) becomes

$$\psi(\mathbf{x}, t + \Delta t) - 2(1 - u^2 D)\psi(\mathbf{x}, t) + \psi(\mathbf{x}, t - \Delta t) = 0. \quad (\text{A7.1.8})$$

Taking $t = \tau \Delta t$ ($\tau = 0, 1, 2, \dots$) and writing $\psi(\mathbf{x}, \tau \Delta t) = \psi_{\tau}$, Eq. (A7.1.8) is equivalent to

$$\psi_{\tau+1} - 2(1 - u^2 D)\psi_{\tau} + \psi_{\tau-1} = 0. \quad (\text{A7.1.9})$$

Postulating a solution of the form

$$\psi_{\tau} = a^{\tau}, \quad (\text{A7.1.10})$$

and inserting this into Eq. (A7.1.9), then dividing by $a^{\tau-1}$, we obtain

$$a^2 - 2(1 - u^2 D)a + 1 = 0. \quad (\text{A7.1.11})$$

We rewrite this as

$$a^2 - 2ba + 1 = 0, \quad (\text{A7.1.12})$$

where

$$b = 1 - u^2 D. \quad (\text{A7.1.13})$$

Solving for a , we find that $a = a_{\pm}$, where

$$a_{\pm} = b \pm \sqrt{b^2 - 1}. \quad (\text{A7.1.14})$$

Because ψ represents an oscillating wave that is not increasing in amplitude, both a_+ and a_- must satisfy

$$|a_{\pm}| \leq 1. \quad (\text{A7.1.15})$$

For any value of $b^2 > 1$, it is easy to see that $|a_+| > 1$ or $|a_-| > 1$, so we must have

$$b^2 \leq 1. \quad (\text{A7.1.16})$$

Thus,

$$a_{\pm} = b \pm i\sqrt{1 - b^2}, \quad (\text{A7.1.17})$$

and hence, $|a_{\pm}|^2 = b^2 + (1 - b^2) = 1$.

Thus, numerically stable oscillatory solutions are guaranteed by the condition given by Eq. (A7.1.16). Inserting the definition of b given by Eq. (A7.1.13) into the stability condition [Eq. (A7.1.16)], we obtain

$$\begin{aligned} 1 - 2u^2 D + u^4 D^2 \leq 1 &\Rightarrow u^2 D \leq 2 \\ &\Rightarrow u^2 \leq \frac{2}{D}, \end{aligned} \quad (\text{A7.1.18})$$

where it is assumed that $u^2 D \neq 0$. The stability condition thus becomes

$$u \leq \sqrt{\frac{2}{D}}. \quad (\text{A7.1.19})$$

What value of D should be used in Eq. (A7.1.19)? The strictest condition is given by the maximum possible value of D , so Eq. (A7.1.19) becomes

$$u \leq \sqrt{\frac{2}{\max(D)}}. \quad (\text{A7.1.20})$$

Examining Eq. (A7.1.7) and using the fact that $0 \leq |1 - \cos\theta| \leq 2$ for all real values of θ , we find that

$$\max(D) = \begin{array}{ll} 2 & \text{in one dimension,} \\ 4 & \text{in two dimensions,} \\ 6 & \text{in three dimensions,} \end{array} \quad (\text{A7.1.21})$$

where $\mathbf{d}^2 = d_x^2$ in one dimension, $\mathbf{d}^2 = d_x^2 + d_y^2$ in two dimensions, and $\mathbf{d}^2 = d_x^2 + d_y^2 + d_z^2$ in three. The stability condition with respect to all k in $d = 1, 2$, or 3 spatial dimensions is thus

$$u \leq u_{\max, S, d} = \frac{\sqrt{d}}{d}. \quad (\text{A7.1.22})$$

Therefore, in the S-FD model, numerical stability is guaranteed by

$$\frac{v \Delta t}{h} \leq \frac{1}{\sqrt{d}}, \quad (\text{A7.1.23})$$

which is called the Courant–Friedrich–Levy (CFL) stability condition.¹⁵

A7.1.2 Nonstandard FDTD

Putting $\tilde{v} \rightarrow u$, which is regarded as a free variable, the NS-FD model of the wave equation is

$$(d_t^2 - u^2 \tilde{\mathbf{d}}^2) \psi(\mathbf{x}, t) = 0, \quad (\text{A7.1.24})$$

where

$$\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \gamma_1 (d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \gamma_2 d_x^2 d_y^2 d_z^2, \quad (\text{A7.1.25})$$

$\gamma_1 = 1/6 + (kh)^2/180$, and $\gamma_2 = 1/30$. Defining $\tilde{D}$ by

$$\tilde{\mathbf{d}}^2 \varphi_k = -2\tilde{D} \varphi_k \quad (\text{A7.1.26})$$

and repeating the previous analysis, we obtain the NS-FDTD stability condition

$$u \leq \sqrt{\frac{2}{\max(\tilde{D})}}. \quad (\text{A7.1.27})$$

We now proceed to determine $\max(\tilde{D})$.

Two dimensions

In two dimensions, $\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \gamma_1 d_x^2 d_y^2$, and using Eqs. (A7.1.5)–(A7.1.7), we find that

$$d_x^2 d_y^2 \varphi_k = 4[1 - \cos(k_x h)][1 - \cos(k_y h)]\varphi_k, \quad (\text{A7.1.28})$$

and hence,

$$\tilde{D} = [1 - \cos(k_x h)] + [1 - \cos(k_y h)] - 2\gamma_1 [1 - \cos(k_x h)][1 - \cos(k_y h)]. \quad (\text{A7.1.29})$$

Differentiating by $k_x h$ and $k_y h$, we find that

$$\frac{\partial}{\partial(k_x h)} \tilde{D} = [2\gamma_1 \cos(k_y h) - 2\gamma_1 + 1] \sin(k_x h), \quad (\text{A7.1.30a})$$

$$\frac{\partial}{\partial(k_y h)} \tilde{D} = [2\gamma_1 \cos(k_x h) - 2\gamma_1 + 1] \sin(k_y h). \quad (\text{A7.1.30b})$$

$\partial_{(k_x h)} \tilde{D} = 0$ if (1) $\cos(k_y h) = (2\gamma_1 - 1)/2\gamma_1$ or (2) $\sin(k_x h) = 0$. Since $-1 \leq \cos(k_y h) \leq 1$ and $\gamma_1 \geq 1/6$, condition (1) cannot be satisfied, and we conclude that an extremum of $\tilde{D}$ occurs at $\sin(k_x h) = 0$. Similarly, setting $\partial_{(k_y h)} \tilde{D} = 0$, we conclude that an extremum of $\tilde{D}$ occurs at $\sin(k_y h) = 0$. Since $\sin(\theta) = 0$ for both $\theta = 0$ and $\theta = \pi$, we compute the second derivatives, $\partial_{(k_x h)}^2 \tilde{D}$, $\partial_{(k_y h)}^2 \tilde{D}$, and $\partial_{(k_y h)} \partial_{(k_x h)} \tilde{D}$, and find that $\partial_{(k_x h)}^2 \tilde{D} < 0$ and $\partial_{(k_y h)}^2 \tilde{D} < 0$ only for $k_x h = k_y h = \pi$ (or odd multiples of π), while $\partial_{(k_y h)} \partial_{(k_x h)} \tilde{D} = 0$ for $\sin(k_x h) = \sin(k_y h) = 0$. Thus, the maximum of $\tilde{D}$ is at $k_x h = k_y h = \pi$. Taking $\gamma_1 = 1/6$, we obtain

$$\max(\tilde{D}) = \frac{8}{3} \quad \text{in two dimensions.} \quad (\text{A7.1.31})$$

Three dimensions

In three dimensions, $\tilde{\mathbf{d}}^2 = \mathbf{d}^2 + \gamma_1 (d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2) + \gamma_2 d_x^2 d_y^2 d_z^2$. Using

$$d_x^2 d_y^2 d_z^2 \varphi_k = -8[1 - \cos(k_x h)][1 - \cos(k_y h)][1 - \cos(k_z h)]\varphi_k, \quad (\text{A7.1.32})$$

we obtain

$$\begin{aligned}
\tilde{D} = & [1 - \cos(k_x h)] + [1 - \cos(k_y h)] \\
& + [1 - \cos(k_z h)] - 2\gamma_1 \{ [1 - \cos(k_x h)][1 - \cos(k_y h)] \\
& + [1 - \cos(k_x h)][1 - \cos(k_z h)] + [1 - \cos(k_y h)][1 - \cos(k_z h)] \} \\
& + 4\gamma_2 [1 - \cos(k_x h)][1 - \cos(k_y h)][1 - \cos(k_z h)].
\end{aligned} \tag{A7.1.33}$$

Following the previous development, we determine $\max(\tilde{D})$. Setting the partial derivatives equal to zero, we find that $\partial_{(k_x h)} \tilde{D} = \partial_{(k_y h)} \tilde{D} = \partial_{(k_z h)} \tilde{D} = 0$ only if $\sin(k_x h) = \sin(k_y h) = \sin(k_z h) = 0$, which implies that $k_x h = k_y h = k_z h = 0$ or π . We then find that $\partial_{(k_x h)}^2 \tilde{D} < 0$, $\partial_{(k_y h)}^2 \tilde{D} < 0$, $\partial_{(k_z h)}^2 \tilde{D} < 0$ only for $k_x h = k_y h = k_z h = \pi$. The mixed partial derivatives are $\partial_{(k_y h)} \partial_{(k_x h)} \tilde{D} = \partial_{(k_z h)} \partial_{(k_x h)} \tilde{D} = \partial_{(k_z h)} \partial_{(k_y h)} \tilde{D} = 0$ for $\sin(k_x h) = \sin(k_y h) = \sin(k_z h) = 0$. Now taking $\gamma_1 = 1/6$ and $\gamma_2 = 1/30$, we obtain

$$\max(\tilde{D}) = \frac{46}{15} \quad \text{in three dimensions.} \tag{A7.1.34}$$

$\tilde{D}$ is a function of both $\mathbf{k}h$ and kh via its dependence on $\gamma_1(kh)$. In both two and three dimensions, we have determined $\max(\tilde{D})$ for $\gamma_1 = \gamma_1(0)$. But Eqs. (A7.1.32) and A7.1.37) give $\max(\tilde{D})$ with respect to all values of $kh > 0$ because $\tilde{D}$ decreases as kh increases in both two and three dimensions.

Inserting the values of $\max(\tilde{D})$ into Eq. (A7.1.27), we obtain the theoretical limits

$$u \leq u_{\max\_NS,2} = \frac{\sqrt{3}}{2} \cong 0.86 \quad \text{in two dimensions,} \tag{A7.1.35a}$$

$$u \leq u_{\max\_NS,3} = \sqrt{\frac{15}{23}} \cong 0.8 \quad \text{in three dimensions.} \tag{A7.1.35b}$$

Note A.7.5.1

This analysis applies to infinite plane waves propagating in a uniform medium. When there are interfaces between different media and computational boundaries, this simple analysis does not necessarily apply. In practical calculations, the stability limits are somewhat lower.

When NS-FDTD is combined with the NS-ABC, the practical stability limits (derived from numerical experiment) become

$$u \leq u_{\max\_NS,2} = 0.80 \quad \text{in two dimensions,} \tag{A7.1.36a}$$

$$u \leq u_{\max\_NS,3} = 0.70 \quad \text{in three dimensions.} \tag{A7.1.36b}$$

Because $u_{\max\_NS,d} > u_{\max\_S,d}$ for $d \geq 2$ for any given wavelength discretization λ/h , the minimum wave period discretization $T/\Delta t$ is smaller in NS-FDTD than in S-FDTD; this implies a larger time step in NS-FDTD than in S-FDTD. Using Eq. (A7.1.36), we find that

$$\frac{T}{\Delta t} \geq \frac{\lambda/h}{0.7} \quad (\text{A7.1.37a})$$

in S-FDTD, and in NS-FDTD,

$$\frac{T}{\Delta t} \geq \frac{\pi}{\arcsin[0.8 \sin(\pi h/\lambda)]}. \quad (\text{A7.1.37b})$$

For example, if $\lambda/h = 10$, then $T/\Delta t \geq 14.3$ in S-FDTD, while in NS-FDTD, $T/\Delta t \geq 12.6$. One could also fix the frequency and set limits on the shortest allowable wavelength.

Designer stability

By adjusting the weights of the difference operators in $\tilde{\mathbf{d}}^2$, it is possible to engineer different values of $u_{\max\_NS}$, but this seems to serve little practical purpose except perhaps in a few special applications.

Higher dimensions and space–time geometry

Formula Eq. (A7.1.23) for S-FDTD stability can be generalized to any number of spatial dimensions. The greater the dimensionality (in Euclidean space) the lower the maximum value of $\nu\Delta t/h$. If space–time is quantized, then the speed of light contains information about its dimensionality.

In NS-FDTD, because diagonal grid points are connected to each other (see Fig. 1.5), the maximum propagation velocity is higher than in S-FDTD. Thus, the speed of light depends not only on the dimensionality of space–time, but also on its geometry.

Whether or not the physical speed of light can actually be used to extract information about space–time dimensionality and geometry is not addressed in this book.

Appendix 7.2 Stability Analysis of the Mur Absorbing Boundary Condition

Let us start with Eq. (7.107a), repeated here,

$$\begin{aligned} \psi_{b,y}^{\tau+1} = & \psi_{b,y}^{\tau} + (\psi_{i,y}^{\tau} - \psi_{i,y}^{\tau-1}) + \left(\frac{1-u_1}{1+u_1} \right) [(\psi_{b,y}^{\tau} - \psi_{b,y}^{\tau-1}) - (\psi_{i,y}^{\tau+1} - \psi_{i,y}^{\tau})] \\ & + \frac{1}{2} \left(\frac{u_2^2}{1+u_1} \right) d_y^2 (\psi_{b,y}^{\tau} + \psi_{i,y}^{\tau}), \end{aligned} \quad (\text{A7.2.1})$$

where $u_1 = \tilde{v}_1$ and $u_2 = \tilde{v}_2$ in the NS-Mur ABC, and $u_1 = u_2 = \nu\Delta t/h$ in the S-Mur ABC. Without loss of generality, we analyze the $b = b_x$ boundary

(where $i = b - 1$) with respect to the infinite plane wave $\psi(x, y, t) = e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}$, where $\mathbf{k} = (k_x, k_y)$, and $\mathbf{x} = (x, y) = (x, y)h$.

Defining $\psi_m^\tau = \psi[(b - 1/2)h, yh, \tau\Delta t]$ as the field midway between the boundary and the interior grid point, $\psi_{b,y}^\tau = \psi(bh, yh, \tau\Delta t)$ and $\psi_{i,y}^\tau = \psi[(b - 1)h, yh, \tau\Delta t]$; therefore, $\psi_{b,y}^\tau = \psi_{m,y}^\tau e^{ik_x h/2}$ and $\psi_{i,y}^\tau = \psi_{m,y}^\tau e^{-ik_x h/2}$. The absorbing boundary condition [Eq. (A7.2.1)] becomes

$$\begin{aligned} \psi_{m,y}^{\tau+1} e^{ik_x h/2} &= \psi_{m,y}^\tau e^{ik_x h/2} + e^{-ik_x h/2} (\psi_{m,y}^\tau - \psi_{m,y}^{\tau-1}) \\ &+ \left(\frac{1 - u_1}{1 + u_1} \right) [e^{ik_x h/2} (\psi_{m,y}^\tau - \psi_{m,y}^{\tau-1}) - e^{-ik_x h/2} (\psi_{m,y}^{\tau+1} - \psi_{m,y}^\tau)] \\ &+ \frac{1}{2} \left(\frac{u_2^2}{1 + u_1} \right) d_y^2 \psi_{m,y}^\tau (e^{ik_x h/2} + e^{-ik_x h/2}). \end{aligned} \quad (\text{A7.2.2})$$

Defining $c_x = \cos(k_x h/2)$, $s_x = \sin(k_x h/2)$, and $s_y^2 = \sin^2(k_y h/2)$; and using $d_y^2 e^{-ik_y y h} / e^{-ik_y y h} = -4s_y^2$, Eq. (A7.2.2) becomes

$$\begin{aligned} e^{ik_x h/2} \psi_{m,y}^{\tau+1} &= 2c_x \psi_{m,y}^\tau - e^{-ik_x h/2} \psi_{m,y}^{\tau-1} \\ &+ \left(\frac{1 - u_1}{1 + u_1} \right) (2c_x \psi_{m,y}^\tau - e^{ik_x h/2} \psi_{m,y}^{\tau-1} - e^{-ik_x h/2} \psi_{m,y}^{\tau+1}) \\ &- 4c_x s_y^2 \left(\frac{u_2^2}{1 + u_1} \right) \psi_{m,y}^\tau. \end{aligned} \quad (\text{A7.2.3})$$

Multiplying both sides by $(1 + u_1)$ and simplifying, we obtain

$$\psi_{m,y}^{\tau+1} = \frac{2c_x(1 - s_y^2 u_2^2 - u_1/2)}{c_x + iu_1 s_x} - \left(\frac{c_x - iu_1 s_x}{c_x + iu_1 s_x} \right) \psi_{m,y}^{\tau-1}. \quad (\text{A7.2.4})$$

Setting $\psi_m^\tau = a^\tau$ to obtain

$$(c_x + iu_1 s_x) a^2 - 2c_x(1 - s_y^2 u_2^2 - u_1/2) a + (c_x - iu_1 s_x) = 0, \quad (\text{A7.2.5})$$

we seek conditions on u_1 and u_2 such that $|a| \leq 1$.

Following Appendix 7.1, we find the condition

$$c_x^2(1 - s_y^2 u_2^2 - u_1/2)^2 \leq c_x^2 + u_1^2 s_x^2 \Rightarrow |a|^2 = 1, \quad (\text{A7.2.6})$$

which reduces to

$$s_y^4 u_2^4 + s_y^2 u_2^2 u_1 - 2s_y^2 u_2^2 + \left(\frac{1}{4} - \frac{s_x^2}{c_x^2} \right) u_1^2 - u_1 \leq 0. \quad (\text{A7.2.7})$$

For the S-Mur ABC, where $u_1 = u_2 = u$, Eq. (A7.2.7) becomes

$$s_y^4 u^4 + s_y^2 u^3 + \left(\frac{1}{4} - 2s_y^2 - \frac{s_x^2}{c_x^2} \right) u^2 - u \leq 0. \quad (\text{A7.2.8})$$

Assuming that $u > 0$, and using $s_y^4 \leq 1$, $s_y^2 \leq 1$, and $s_x^2/c_x^2 \geq 0$, taking the maximum value of the left side of Eq. (A7.2.8) yields

$$u^4 + u^3 + \frac{1}{4}u^2 - u \leq 0 \quad \Rightarrow \quad (\text{A7.2.9a})$$

$$u^3 + u^2 + \frac{1}{4}u \leq 1. \quad (\text{A7.2.9b})$$

Defining $\eta_2 = (\sqrt{330}/36 + 109/216)^{1/3}$, Eq. (A7.2.9b) gives the condition

$$u \leq \eta_2 + \frac{1}{36\eta_2} - \frac{1}{3} = 0.697^+. \quad (\text{A7.2.10})$$

As noted in Section 7.5.4, the practical limit (with a safety margin) is as follows:

Stability of the S-Mur ABC in two dimensions:

$$u = \frac{v\Delta t}{h} \leq 0.67. \quad (\text{A7.2.11})$$

This limit is slightly below the analytic stability limit of S-FDTD for the wave equation, $v\Delta t/h \leq 0.70$.

In three dimensions, Eq. (A7.2.1) becomes

$$\begin{aligned} \psi_{b,y}^{\tau+1} = & \psi_{b,y,z}^{\tau} + (\psi_{i,y,z}^{\tau} - \psi_{i,y,z}^{\tau-1}) + \left(\frac{1-u_1}{1+u_1} \right) [(\psi_{b,y,z}^{\tau} - \psi_{b,y,z}^{\tau-1}) \\ & - (\psi_{i,y,z}^{\tau+1} - \psi_{i,y,z}^{\tau})] + \frac{1}{2} \left(\frac{u_2^2}{1+u_1} \right) (d_y^2 + d_z^2) (\psi_{b,y,z}^{\tau} + \psi_{i,y,z}^{\tau}), \end{aligned} \quad (\text{A7.2.12})$$

and $\mathbf{k} = (k_x, k_y, k_z)$. Putting $s_y^2 \rightarrow s_y^2 + s_z^2$, where $s_z = \sin(k_z h/2)$, in Eq. (A7.2.7), the equation becomes

$$(s_y^2 + s_z^2)^2 u_2^4 + (s_y^2 + s_z^2) u_2^2 u_1 - 2(s_y^2 + s_z^2) u_2^2 + \left(\frac{1}{4} - \frac{s_x^2}{c_x^2} \right) u_1^2 - u_1 \leq 0. \quad (\text{A7.2.13})$$

Taking $u_1 = u_2 = u$, Eq. (A7.2.13) becomes

$$(s_y^2 + s_z^2)^2 u^4 + (s_y^2 + s_z^2) u^3 + \left[\frac{1}{4} - 2(s_y^2 + s_z^2) - \frac{s_x^2}{c_x^2} \right] u^2 - u \leq 0, \quad (\text{A7.2.14})$$

and taking the maximum value of the left side of Eq. (A7.2.14) yields the condition

$$4u^4 + 2u^3 + \frac{1}{4}u^2 - u \leq 0 \quad \Rightarrow \quad (\text{A7.2.15a})$$

$$4u^3 + 2u^2 + \frac{1}{4}u \leq 1. \quad (\text{A7.2.15b})$$

Defining $\eta_3 = (\sqrt{327}/144 + 217/1728)^{1/3}$, we obtain the stability limit

$$u \leq \eta_3 + \frac{1}{144\eta_3} - \frac{1}{6} = 0.475^+. \quad (\text{A7.2.16})$$

A practical limit with a margin of safety is as follows:

Stability of the S-Mur ABC in three dimensions:

$$u = \frac{v\Delta t}{h} \leq 0.45. \quad (\text{A7.2.17})$$

Note that this is somewhat lower than the analytical stability limit of S-FDTD for the wave equation, $v\Delta t/h \leq 0.57$.

Stability of the S-Mur ABC in two dimensions

The stability analysis of the NS-Mur ABC is much more complicated because there are two independent variables, $u_1 \neq u_2$. In principle, the analysis could be reduced to one variable because $\tilde{v}_1$ and $\tilde{v}_2$ are connected via Eq. (7.106), but the relationship is too complicated to analyze.

Assuming that both $u_1 > 0$ and $u_2 > 0$, clearly, taking $s_x^2/c_x^2 = 0$ maximizes the left side of Eq. (A7.2.7), but it is not obvious whether $s_y^2 = 0$ or $s_y^2 = 1$ gives a maximum. Inserting the actual numerical values of $\tilde{v}_1$ and $\tilde{v}_2$ used in working algorithms, we find that taking $s_y^2 = 0$ yields the maximum (but negative value) and gives the condition $u_1 < 4$ for arbitrary values of u_2^2 . Taking $s_y^2 = 1$ yields

$$u_2^4 + u_2^2 u_1 - 2u_2^2 + \frac{1}{4}u_1^2 - u_1 \leq 0, \quad (\text{A7.2.18})$$

which is somewhat greater, but still negative for all practical algorithms. This expression gives a limit on u_2^2 that can be found numerically for any given u_1 .

Stability of the NS-Mur ABC in three dimensions

In three dimensions, using Eq. (A7.2.13), we can do a similar analysis to obtain

$$\frac{1}{4}u_1^2 - u_1 \leq 0, \quad (\text{A7.2.19})$$

$$4u_2^4 + 2u_2^2u_1 - 4u_2^2 + \frac{1}{4}u_1^2 - u_1 \leq 0. \quad (\text{A7.2.20})$$

For all practical algorithms, we have found that these conditions are satisfied and yield numerical stability. In three dimensions, we can perform a similar analysis. Thus, the NS-FDTD stability limits confirmed by numerical experiment become the following:

Stability of the NS-Mur ABC in two and three dimensions:

$$\tilde{\nu} \leq 0.80 \quad \text{in two dimensions,}$$

$$\tilde{\nu} \leq 0.70 \quad \text{in three dimensions.}$$

Devil in the details

This analysis is with respect to an infinite plane wave impinging on an infinitely long computational boundary. If the ABC is not properly implemented at the corners, it can be numerically unstable.

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Chapter 8

Review of Electromagnetic Theory

We begin with a brief review of electromagnetic theory, and then derive analytic solutions to a few interesting problems. Although few analytic solutions exist, those that do are of great interest because they allow us to check numerical algorithms and often yield interesting physical insights that numerical solutions alone cannot. A sound theoretical understanding of analytic techniques is essential to comprehend numerical computations and to understand their limitations.

8.1 Maxwell's Equations: General Formulation

Let $\mathbf{B}$ be the magnetic induction, $\mathbf{H}$ the magnetic field, $\mathbf{D}$ the electric displacement, $\mathbf{E}$ the electric field, ρ the charge density, and $\mathbf{J}$ the electric current density. All of these quantities are functions of position $\mathbf{x}$ and time t . We write Maxwell's equations in the form

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}, \quad (8.1)$$

$$\partial_t \mathbf{D} = \nabla \times \mathbf{H} - \mathbf{J}, \quad (8.2)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (8.3)$$

$$\nabla \cdot \mathbf{D} = \rho. \quad (8.4)$$

Different authors insert different constants into Maxwell's equations depending on the system of units employed. We have chosen this form because it is convenient for computational purposes. Computations can be readily compared with physical measurements by scaling the results.

The last two of Maxwell's equations are related to the first two. Taking the divergence of both sides of Eq. (8.1), we obtain

$$\begin{aligned}\partial_t(\nabla \bullet \mathbf{B}) &= -\nabla \bullet (\nabla \times \mathbf{E}) \\ &= 0\end{aligned}\quad (8.5)$$

using the identity

$$\nabla \bullet (\nabla \times \mathbf{V}) = 0, \quad (8.6)$$

which holds for any vector field $\mathbf{V}$. Integrating Eq. (8.5) with respect to time, we find that $\nabla \bullet \mathbf{B} = \text{a constant}$. A nonzero value of this constant would imply the existence of magnetic charge (magnetic monopoles) analogous to electric charge or a background magnetic field. Currently, there is no experimental evidence for either so we take $\nabla \bullet \mathbf{B} = 0$. Equation (8.1) does not contain a magnetic charge current because none has been observed.

Note 8.1

Absence of evidence is not evidence of absence, however, so the search for magnetic monopoles continues. In certain systems, entities that behave like magnetic monopoles have been reported, but so far, unlike electric charge (an electric monopole), no free magnetic monopoles have been found. Further discussion of this topic can be found in the current physics literature; see, for example, Ref. 1.

Similarly, Eq. (8.2) implies Eq. (8.4). Taking the divergence of both sides of Eq. (8.2) and using Eq. (8.6) yields

$$\partial_t(\nabla \bullet \mathbf{D}) = -\nabla \bullet \mathbf{J}. \quad (8.7)$$

Volume integrating both sides, and using the divergence theorem on the right, we obtain

$$\partial_t \int_V \nabla \bullet \mathbf{D} = - \int_V \nabla \bullet \mathbf{J} = - \oint_S \mathbf{ds} \bullet \mathbf{J}, \quad (8.8)$$

where V is a volume bounded by a closed surface S ; $dv (= dxdydz$ in Cartesian coordinates) is an infinitesimal volume element; and $ds = |ds|$ is an infinitesimal surface element, where $ds = \hat{\mathbf{n}}ds$, and $\hat{\mathbf{n}}$ is a unit vector normal to S and which points outwards from V .

Since electric charge is conserved, the charge flowing out of V , given by the second integral on right side of Eq. (8.8), must equal the rate of decrease of charge within V , given by the left side of the equation. Thus,

$$\oint_S \mathbf{ds} \bullet \mathbf{J} = -\partial_t \int_V dv \rho, \quad (8.9)$$

which is the continuity equation for charge (another statement of charge conservation).

Comparing Eqs. (8.8) and (8.9), we find that

$$\partial_t \nabla \bullet \mathbf{D} = \partial_t \rho. \quad (8.10)$$

Integrating both sides with respect to time, we find that $\nabla \bullet \mathbf{D} = \rho +$ a constant. Mathematically, it is possible that this constant is nonzero, but this would imply that there is some background $\mathbf{D}$ field that exists in the absence of charge. There is no experimental evidence for this, so we conclude that this constant $= 0$, leaving $\nabla \bullet \mathbf{D} = \rho$. Thus Maxwell's second equation [Eq. (8.2)] implies the last [Eq. (8.4)].

We are now left with two equations, Eqs. (8.1) and (8.2), that relate six unknown fields: $\mathbf{B}$, $\mathbf{H}$, $\mathbf{D}$, $\mathbf{E}$, $\mathbf{J}$, and ρ . Therefore, to actually solve Maxwell's equations, additional relationships between these fields are needed. These relationships ultimately derive from experiment. Actual physical media can be very complicated, but often their essential properties can be extracted and idealized, and the resulting set of equations can be an excellent approximation to reality.

8.2 Linear Media

Linear media are the simplest of all. If the macroscopic electric and magnetic fields are weak (compared with the microscopic fields that act within and between atoms and molecules), then it is an excellent approximation to take

$$\mathbf{B} = \mu \mathbf{H}, \quad (8.11)$$

$$\mathbf{D} = \varepsilon \mathbf{E}, \quad (8.12)$$

where the magnetic permeability μ and the electrical permittivity ε are constant with respect to time but not necessarily position. The simplest medium of all is vacuum, where $\varepsilon = \varepsilon_0$, and $\mu = \mu_0$. In this book we employ a system of units in which

$$\varepsilon_0 = 1 \quad (8.13)$$

in vacuum. This implies that

$$\mu_0 = 1/c^2, \quad (8.14)$$

where c is the vacuum velocity of light.

Note 8.2

On occasion we let $\varepsilon_0 = 1$ denote the permittivity of the ambient medium in which an object of interest (for example, a scatterer) is immersed. If the velocity of light in the ambient medium is v_0 , then $\mu_0 = 1/v_0^2$.

Except in plasmas, most matter is macroscopically electrically neutral, so the density of free charge is zero. Thus, we can usually take

$$\rho = 0. \quad (8.15)$$

Next, we need a relationship between the electric current and the electromagnetic fields. For analytical purposes it is convenient to decompose the electric current into two parts,

$$\mathbf{J} = \mathbf{J}_s + \mathbf{J}_c, \quad (8.16)$$

where $\mathbf{J}_s$ is an external source current (we can regard it as magically inserted by some demiurge), and $\mathbf{J}_c$ is the conduction current, which is produced by the electromagnetic fields within the region of interest. In general, $\mathbf{J}_c = \mathbf{J}_c(\mathbf{E}, \mathbf{B})$, but in many materials the conduction current is a linear function of the electric field, and we can take

$$\mathbf{J}_c = \sigma \mathbf{E}, \quad (8.17)$$

where the conductivity σ is a function of position but not of time. Except in media such as plasmas, where the conduction current is strongly affected by magnetic fields, Eq. (8.17) is a good model. In ordinary conductors, due to the Hall effect, $\mathbf{J}_c$ is affected by the magnetic field, but this effect is usually very small and can be neglected.

Equations (8.11), (8.12), (8.15), and (8.17) define the idealized linear medium with which we deal.

8.2.1 Maxwell's equations in a linear nonconducting medium with no source current

Taking $\sigma = 0$ defines a linear nonconducting medium; assuming that there is no free charge and taking $\mathbf{J}_s = 0$, Maxwell's Eqs. (8.1) and (8.2) simplify to

$$\mu \partial_t \mathbf{H} = -\nabla \times \mathbf{E}, \quad (8.18)$$

$$\varepsilon \partial_t \mathbf{E} = \nabla \times \mathbf{H}, \quad (8.19)$$

and Maxwell's Eqs. (8.3) and (8.4) reduce to

$$\nabla \cdot (\varepsilon \mathbf{E}) = 0, \quad (8.20)$$

$$\nabla \cdot (\mu \mathbf{H}) = 0. \quad (8.21)$$

For further analysis, we use the identities

$$\nabla \cdot (\varphi \mathbf{V}) = \varphi \nabla \cdot \mathbf{V} + \mathbf{V} \cdot \nabla \varphi, \quad (8.22)$$

$$\nabla \times (\nabla \times \mathbf{V}) = \nabla(\nabla \cdot \mathbf{V}) - \nabla^2 \mathbf{V}, \quad (8.23)$$

$$\nabla \times (\varphi \mathbf{V}) = \varphi \nabla \times \mathbf{V} + \mathbf{V} \times \nabla \varphi, \quad (8.24)$$

which hold for arbitrary scalar and vector fields $\varphi = \varphi(\mathbf{x})$ and $\mathbf{V} = \mathbf{V}(\mathbf{x})$.

Applying identity Eq. (8.22) to Eqs. (8.20) and (8.21), we obtain

$$\varepsilon \nabla \bullet \mathbf{E} + \mathbf{E} \bullet \nabla \varepsilon = 0, \quad (8.25)$$

$$\mu \nabla \bullet \mathbf{H} + \mathbf{H} \bullet \nabla \mu = 0. \quad (8.26)$$

Thus, at the boundaries between media, where $\nabla \varepsilon \neq 0$ and $\nabla \mu \neq 0$, we have $\nabla \bullet \mathbf{E} \neq 0$ and $\nabla \bullet \mathbf{H} \neq 0$, but in a uniform medium we have $\nabla \varepsilon = 0 \Rightarrow \nabla \bullet \mathbf{E} = 0$ and $\nabla \mu = 0 \Rightarrow \nabla \bullet \mathbf{H} = 0$.

We now derive wave equations for $\mathbf{E}$ and $\mathbf{H}$. Multiplying Eq. (8.18) by ε , differentiating by t , and using Eq. (8.19) yields

$$\varepsilon \mu \partial_t^2 \mathbf{H} = -\varepsilon \nabla \times \left(\frac{1}{\varepsilon} \nabla \times \mathbf{H} \right). \quad (8.27)$$

Employing identity Eqs. (8.22)–(8.24), Eq. (8.7) can be cast in the form

$$\left(\partial_t^2 - \frac{1}{\varepsilon \mu} \nabla^2 \right) \mathbf{H} = \frac{1}{\mu} \nabla \left(\frac{1}{\varepsilon} \right) \times (\nabla \times \mathbf{H}) - \frac{1}{\varepsilon \mu} \nabla (\nabla \bullet \mathbf{H}). \quad (8.28)$$

Similarly, multiplying Eq. (8.19) by μ , differentiating by t , and using Eq. (8.18) yields

$$\left(\partial_t^2 - \frac{1}{\varepsilon \mu} \nabla^2 \right) \mathbf{E} = \frac{1}{\varepsilon} \nabla \left(\frac{1}{\mu} \right) \times (\nabla \times \mathbf{E}) - \frac{1}{\varepsilon \mu} \nabla (\nabla \bullet \mathbf{E}). \quad (8.29)$$

Away from the boundaries between different media, within a uniform region in which ε and μ are neither functions of position nor of time,

$$\nabla \bullet \mathbf{E} = 0, \quad (8.30)$$

$$\nabla \bullet \mathbf{H} = 0. \quad (8.31)$$

Substituting Eq. (8.30) into Eq. (8.28), and Eq. (8.31) into Eq. (8.29), we obtain independent wave equations for $\mathbf{E}$ and $\mathbf{H}$:

$$\left(\partial_t^2 - \frac{1}{\varepsilon \mu} \nabla^2 \right) \mathbf{H} = 0, \quad (8.32)$$

$$\left(\partial_t^2 - \frac{1}{\varepsilon \mu} \nabla^2 \right) \mathbf{E} = 0. \quad (8.33)$$

In Chapter 4 we showed that the general solution to the wave equation is given by $\psi(x, t) = f(x \mp vt)$, where v is the velocity of the waves. Thus, in free

space we make the identification $c = 1/\epsilon_0\mu_0$, where c is the velocity of light in vacuum. Because we have set $\epsilon_0 = 1$, $\mu_0 = 1/c^2$. In a medium where the velocity of light is

$$v = \frac{c}{n}, \quad (8.34)$$

it follows that

$$v^2 = \frac{1}{\epsilon\mu}, \quad (8.35)$$

$$n^2 = \frac{\epsilon\mu}{\mu_0}. \quad (8.36)$$

Except for ferromagnetic materials, it is often an excellent approximation to take $\mu = \mu_0$ everywhere; thus, $n^2 = \epsilon$, where n is the refractive index.

Although in Maxwell's equations they are coupled together, the preceding analysis seems to show that that Maxwell's equations [Eqs. (8.18) and (8.19)] are equivalent to two independent wave equations in $\mathbf{H}$ and $\mathbf{E}$. As we noted in Section 3.3, however, when a differential equation is differentiated [for example, $y'(x)=0 \rightarrow y''(x)=0$], the new equation is not equivalent to the original equation and has additional solutions. The lower-order equation implies the higher-order one, but not vice versa. Maxwell's equations imply the wave equation, but Maxwell's equations cannot be derived from the wave equation.

8.2.2 Maxwell's equations in a linear conducting medium with a source current

Assuming no free charge, and taking $\sigma \neq 0$, $\mathbf{J}_s \neq 0$ in a region of constant ϵ and μ , Maxwell's equations become

$$\mu\partial_t\mathbf{H} = -\nabla \times \mathbf{E}, \quad (8.37)$$

$$\epsilon\partial_t\mathbf{E} = \nabla \times \mathbf{H} - \sigma\mathbf{E} - \mathbf{J}_s. \quad (8.38)$$

Now multiplying Eq. (8.37) by ϵ , differentiating by t , and using Eq. (8.38) yields

$$\left(\partial_t^2 + \frac{\sigma}{\epsilon}\partial_t - \frac{1}{\epsilon\mu}\nabla^2\right)\mathbf{H} = \frac{1}{\epsilon\mu}\nabla \times \mathbf{J}_s. \quad (8.39)$$

Similarly, multiplying Eq. (8.38) by μ , differentiating by t , and using Eq. (8.37) yields

$$\left(\partial_t^2 + \frac{\sigma}{\epsilon} \partial_t - \frac{1}{\epsilon \mu} \nabla^2 \right) \mathbf{E} = -\frac{1}{\epsilon} \partial_t \mathbf{J}_s. \quad (8.40)$$

Comparing Eq. (8.39) with the absorbing wave equation [Eq. (4.78)], we make the identifications

$$\frac{\sigma}{2\epsilon} = \alpha, \quad (8.41)$$

$$-\frac{1}{\epsilon} \partial_t \mathbf{J}_s = \mathbf{s}, \quad (8.42)$$

where $\mathbf{s}$ is now a vector source.

Conductivity, dispersion, and complex electrical permittivity

As we noted in Chapter 4, adding absorption to the wave equation gives rise to dispersive effects, and absorption can be incorporated into a complex index of refraction. Similarly, conductivity gives rise to dispersive behavior, and conductivity can be incorporated into a complex permittivity. If the time dependence of the frequency component $\mathbf{E}_\omega$ of $\mathbf{E}$ is taken to be $e^{i\omega t}$, then taking $\mathbf{J}_s = 0$ in Eq. (8.38), Eq. (8.38) becomes

$$i\omega (\epsilon - i\sigma/\omega) \mathbf{E}_\omega = \nabla \times \mathbf{H}_\omega, \quad (8.43)$$

which can be expressed as

$$(\epsilon - i\sigma/\omega) \partial_t \mathbf{E}_\omega = \nabla \times \mathbf{H}_\omega; \quad (8.44)$$

thus,

$$\hat{\epsilon} = (\epsilon - i\sigma/\omega) \quad (8.45)$$

is the complex permittivity.

Devil in the details

If the time dependence is taken to be $e^{-i\omega t}$, then $\hat{\epsilon} = (\epsilon + i\sigma/\omega)$.

Thus, because of conductivity (although this is not the only reason), metals are dispersive materials. As we shall later see, computing light propagation in dispersive materials is much more difficult than in nondispersive ones. Actually, all materials are dispersive, but at sufficiently low frequencies, dispersion can often be neglected. The concept of complex permittivity is further developed in Section 8.5.

8.3 Boundary Conditions

On the interface between two different media, the electromagnetic fields must satisfy certain conditions. Electromagnetic boundary conditions are derived in many excellent texts, such as Refs. 2 and 3, so here we merely state those conditions that are relevant for our purposes.

Let $\mathbf{x}_B$ be a point on the boundary B between two media, $\hat{\mathbf{n}}$ a unit vector normal to B , and $\hat{\mathbf{t}}$ a unit vector tangent to B (hence, perpendicular to $\hat{\mathbf{n}}$). We assume that there are no currents on the boundary and no free charge. Taking the electromagnetic fields in media 1 and 2 to be $(\mathbf{E}_{1,2}, \mathbf{H}_{1,2})$, respectively, the tangential components of $\mathbf{E}$ and $\mathbf{H}$ must be continuous across the boundary; thus,

$$\hat{\mathbf{t}} \cdot \mathbf{E}_1(\mathbf{x}_B, t) = \hat{\mathbf{t}} \cdot \mathbf{E}_2(\mathbf{x}_B, t), \quad (8.46a)$$

$$\hat{\mathbf{t}} \cdot \mathbf{H}_1(\mathbf{x}_B, t) = \hat{\mathbf{t}} \cdot \mathbf{H}_2(\mathbf{x}_B, t). \quad (8.46b)$$

These are the boundary conditions most often encountered in optics, where surface current and charge density vanish or can be neglected.

8.4 Linear Dispersive Materials

8.4.1 Constitutive relations

In a dielectric material let $\mathbf{D} = \mathbf{E} = 0$ for $t \leq 0$; now, assume that we turn on an externally applied electric field at $t = 0$. The electrons move in response and give rise to a polarization field $\mathbf{P}_E$ that opposes $\mathbf{E}$; thus, $\mathbf{D} = \mathbf{E} + \mathbf{P}_E$ can be interpreted as the electric field that *would* exist if there were no polarization. In a linear dielectric,

$$\mathbf{P}_E = \chi_E \mathbf{E}, \quad (8.47)$$

where χ_E is the electric susceptibility. Thus,

$$\varepsilon = 1 + \chi_E. \quad (8.48)$$

Because the electrons cannot respond instantaneously to the applied electric field, the polarization is actually a function of time so that $\mathbf{P}_E = \mathbf{P}_E(t)$ —the spatial dependence is omitted for simplicity. The relaxation time τ is the time needed for the polarization of a material to reach equilibrium with a steady $\mathbf{E}$ field. Then χ_E is a constant for $t > \tau$, and Eq. (8.47) holds. If $\mathbf{E}$ oscillates with period $T \gg \tau$, χ_E can also be regarded as a constant, and Eq. (8.47) is an excellent approximation; however, if $T < \tau$, then $\chi_E = \chi_E(t)$, and $\mathbf{P}_E(t) \neq \chi_E(t)\mathbf{E}(t)$. Hence, $\mathbf{D}(t) \neq \varepsilon(t)\mathbf{E}(t)$.

For the same reason, the magnetic polarization $\mathbf{P}_M$ is no longer simply related to the magnetic susceptibility when the oscillation period is less than the relaxation time, and $\mathbf{P}_M(t) \neq \chi_M(t)\mathbf{H}(t)$, $\mathbf{B}(t) \neq \mu(t)\mathbf{H}(t)$; similarly, $\mathbf{J}_c(t) \neq \sigma(t)\mathbf{E}(t)$.

However, in the frequency domain,

$$\tilde{\mathbf{P}}_{\text{E}}(\omega) = \tilde{\chi}_{\text{E}}(\omega)\tilde{\mathbf{E}}(\omega), \quad (8.49)$$

where the “ $\sim$ ” overscript denotes the Fourier transform. Thus,

$$\tilde{\mathbf{D}}(\omega) = \tilde{\epsilon}(\omega)\tilde{\mathbf{E}}(\omega), \quad (8.50)$$

and similarly,

$$\tilde{\mathbf{B}}(\omega) = \tilde{\mu}(\omega)\tilde{\mathbf{H}}(\omega), \quad (8.51)$$

$$\tilde{\mathbf{J}}_{\text{c}}(\omega) = \tilde{\sigma}(\omega)\tilde{\mathbf{E}}(\omega). \quad (8.52)$$

Fourier transform

Any “reasonable” function of time $f(t)$ can be expressed in terms of its Fourier transform $\tilde{f}(\omega)$ by

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \tilde{f}(\omega), \quad (8.53)$$

where

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t} f(t). \quad (8.54)$$

Equation (8.54) defines the Fourier transform operation $\mathbf{F}$ on function f , for which we write $\tilde{f} = \mathbf{F}[f]$; Eq. (8.53) defines the inverse Fourier transform operation $\mathbf{F}^{-1}$, which acts on $\tilde{f}$, and for which we write $f = \mathbf{F}^{-1}[\tilde{f}]$. The most important properties of the Fourier transform are derived and summarized in Appendix 8.1.

Applying the Fourier convolution theorem (see Appendix 8.1),

$$\begin{aligned} \mathbf{F}^{-1}[\tilde{f} \tilde{g}] &= \int_{-\infty}^{\infty} dt' f(t) g(t - t') \\ &= \int_{-\infty}^{\infty} dt' g(t) f(t - t'), \end{aligned} \quad (8.55)$$

to the frequency domain constitutive relations [Eqs. (8.50)–(8.52)], we obtain

$$\mathbf{D}(t) = \int_0^t dt' \epsilon(t') \mathbf{E}(t - t'), \quad (8.56)$$

$$\mathbf{B}(t) = \int_0^t dt' \mu(t') \mathbf{H}(t - t'), \quad (8.57)$$

$$\mathbf{J}_{\text{c}}(t) = \int_0^t dt' \sigma(t') \mathbf{E}(t - t'). \quad (8.58)$$

The integration limits in Eqs. (8.56)–(8.58) are a consequence of causality: $\mathbf{E}$ causes $\mathbf{D}$ and $\mathbf{J}_c$, and $\mathbf{H}$ causes $\mathbf{B}$. Assuming that the electromagnetic field vanishes for $t \leq 0$, $\mathbf{D}$ is produced by the action of $\mathbf{E}$ starting from time $= 0$ (when $\mathbf{E}$ is turned on) to time $= t$. $\mathbf{D}$ cannot be affected by values of $\mathbf{E}$ at time $\geq t$. In other words, the future cannot affect the past, but past history does determine the future. Similar considerations hold for $\mathbf{B}$ and $\mathbf{J}_c$. This is the principle of causality.

Constant permittivity in the frequency domain

Now suppose that $\tilde{\epsilon}(\omega) = \epsilon = \text{a constant}$. Taking the inverse Fourier transform, $\epsilon = \mathbf{F}^{-1}[\tilde{\epsilon}]$, and using Eq. (A8.1.4), we obtain

$$\epsilon(t) = \epsilon \delta(t). \quad (8.59)$$

Inserting Eq. (8.59) into Eq. (8.56) gives

$$\mathbf{D}(t) = \epsilon \mathbf{E}(t), \quad (8.60)$$

which is the same as Eq. (8.12) for nondispersive linear media. If $\tilde{\epsilon}(\omega)$ is a constant, then $\epsilon(t)$ is a δ function. A δ function is infinitesimally narrow, which means that the response time τ vanishes. Thus, when τ is negligible, $\mathbf{D}(t) = \epsilon \mathbf{E}(t)$, where ϵ is constant. The response time τ is negligible if it is small compared to the wave period (frequency $\ll 1/\tau$). In a physical material, when the frequency is much larger than the highest resonance frequency, the response decreases with frequency because the system does not have enough time to respond to the applied field. On physical grounds, we thus expect that

$$\lim_{\omega \rightarrow \infty} \tilde{\epsilon}(\omega) = 0. \quad (8.61)$$

Note 8.3

To derive Eq. (8.60) we must use the full form of the convolution theorem [Eq. (8.55)]:

$$\mathbf{D}(t) = \epsilon \int_{-\infty}^{\infty} dt' \delta(t') \mathbf{E}(t - t') = \epsilon \mathbf{E}(t). \quad (8.62)$$

Most materials are dispersive, but if $\tilde{\epsilon}$, $\tilde{\mu}$, and $\tilde{\sigma}$ are nearly constant over a wide frequency band centered on ω_0 , then dispersion can be neglected for frequencies in this band, and Eqs. (8.37) and (8.38) are excellent models of electromagnetism.

Constant permittivity in the time domain

Now let $\epsilon(t) = \epsilon = \text{a constant}$. Taking the Fourier transform, we find that

$$\tilde{\epsilon}(\omega) = 2\pi\epsilon\delta(\omega). \quad (8.63)$$

This implies that the frequency domain permittivity is nonvanishing only at frequency = 0, which corresponds to infinite periodicity.

Substituting $\epsilon(t) = \epsilon$ into Eq. (8.56) gives

$$\mathbf{D}(t) = \epsilon \int_0^t dt' \mathbf{E}(t - t'). \quad (8.64)$$

If $\mathbf{E}(t) = \mathbf{E} = \text{a constant} > 0$ for $t > 0$, and $\mathbf{E}(t) = 0$ for $t \leq 0$, then

$$\mathbf{D}(t) = \epsilon \mathbf{E} t \quad (8.65)$$

for $t > 0$. This tells us that the polarization continues to increase without reaching saturation. In other words, the response time is infinite. This follows from Eq. (8.63) because the periodicity of $\tilde{\epsilon}(0)$ is infinite.

8.4.2 Maxwell's equations

Inserting the constitutive relations Eqs. (8.56)–(8.58) into Maxwell's Eqs. (8.1)–(8.2), the latter become

$$\partial_t \int_0^t dt' \mu(t') \mathbf{H}(t - t') = -\nabla \times \mathbf{E}(t), \quad (8.66)$$

$$\partial_t \int_0^t dt' \epsilon(t') \mathbf{E}(t - t') = \nabla \times \mathbf{H}(t) - \int_0^t dt' \sigma(t') \mathbf{E}(t - t') - \mathbf{J}_s(t). \quad (8.67)$$

The $\mathbf{x}$ dependence is omitted for notational simplicity.

Thus, in dispersive materials, in the time domain, Maxwell's equations become integro-differential equations, which are challenging to solve both analytically and numerically.

Ultimately we need models of dispersive permittivity and permeability to solve Maxwell's equations. See Chapter 12 for models used for optical frequencies, and references 16 and 17 of Chapter 2 for an interesting model using noninteger derivatives in the terahertz and infrared regimes.

8.5 Kramers–Kronig Relations

Without modeling material properties, much can be learned by a very general mathematical analysis of dispersive electric permittivity (and magnetic permeability). The Kramers–Kronig relations^{2,3} not only yield useful theoretical insights but also give practical expressions relating the real and complex parts of the permittivity independently of any particular physical model.

Taking the inverse Fourier transform of Eq. (8.50), we have

$$\mathbf{D}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \tilde{\varepsilon}(\omega) \tilde{\mathbf{E}}(\omega). \quad (8.68)$$

By definition,

$$\tilde{\mathbf{E}}(\omega) = \int_{-\infty}^{\infty} dt' e^{-i\omega t'} \mathbf{E}(t'). \quad (8.69)$$

Substituting Eq. (8.69) into Eq. (8.68), we obtain

$$\begin{aligned} \mathbf{D}(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \tilde{\varepsilon}(\omega) \int_{-\infty}^{\infty} dt' e^{-i\omega t'} \mathbf{E}(t') \\ &= \int_{-\infty}^{\infty} dt' \mathbf{E}(t') \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t')} \tilde{\varepsilon}(\omega). \end{aligned} \quad (8.70)$$

Defining $\tilde{\chi}(\omega) = \tilde{\varepsilon}(\omega) - \varepsilon_0$, where ε_0 is a constant, we then have

$$\chi(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega\tau} \tilde{\chi}(\omega). \quad (8.71)$$

Using Eq. (A8.1.4) and $\tilde{\varepsilon}(\omega) = \varepsilon_0 + \tilde{\chi}(\omega)$, Eq. (8.70) becomes

$$\begin{aligned} \mathbf{D}(t) &= \int_{-\infty}^{\infty} dt' \mathbf{E}(t') \chi(t-t') + \int_{-\infty}^{\infty} dt' \mathbf{E}(t') \varepsilon_0 \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t')} \\ &= \varepsilon_0 \mathbf{E}(t) + \int_{-\infty}^{\infty} dt' \mathbf{E}(t') \chi(t-t'). \end{aligned} \quad (8.72)$$

From the principle of causality (see Section 8.4), $\mathbf{D}(t)$ can only depend on $\mathbf{E}(t')$ for $t' \leq t$; thus,

$$\chi(\tau) = 0 \text{ for } \tau < 0, \quad (8.73)$$

and Eq. (8.72) becomes

$$\mathbf{D}(t) = \varepsilon_0 \mathbf{E}(t) + \int_0^t dt' \mathbf{E}(t') \chi(t-t'). \quad (8.74)$$

Taking both $\mathbf{D}(t)$ and $\mathbf{E}(t)$ to be real, $\chi(t-t')$ must also be real. Now let χ be any real function that satisfies causality Eq. (8.73) and for which the integral in Eq. (8.74) exists. Taking the Fourier transform of Eq. (8.71), and using causality, we find that

$$\tilde{\chi}(\omega) = \int_0^{\infty} d\tau e^{-i\omega\tau} \chi(\tau); \quad (8.75)$$

thus,

$$\tilde{\varepsilon}(\omega) = \varepsilon_0 + \int_0^{\infty} d\tau e^{-i\omega\tau} \chi(\tau). \quad (8.76)$$

Because, in general, $\tilde{\epsilon}(\omega)$ is complex but $\chi(\tau)$ and ϵ_0 are real,

$$\begin{aligned}\tilde{\epsilon}^*(\omega) &= \epsilon_0 + \int_0^\infty d\tau e^{i\omega\tau} \chi(\tau) \\ &= \tilde{\epsilon}(-\omega).\end{aligned}\quad (8.77)$$

Decomposing $\tilde{\epsilon}$ into real and imaginary parts, $\tilde{\epsilon}(\omega) = \tilde{\epsilon}_r(\omega) + i\tilde{\epsilon}_i(\omega)$, we find from Eq. (8.77) that

$$\tilde{\epsilon}_r(-\omega) = \tilde{\epsilon}_r(\omega), \quad (8.78a)$$

$$\tilde{\epsilon}_i(-\omega) = -\tilde{\epsilon}_i(\omega). \quad (8.78b)$$

Thus, $\tilde{\epsilon}_r(\omega)$ is an even function, and $\tilde{\epsilon}_i(\omega)$ is an odd function.

Let us now extend $\tilde{\chi}(\omega)$ into the complex plane by putting $\tilde{\chi}(\omega) \rightarrow \tilde{\chi}(z)$. Next, we define the contour integral

$$I_C = \oint_C dz \frac{\tilde{\chi}(z)}{z - \omega} \quad (8.79)$$

on the closed contour C shown in Fig. 8.1. Since the integrand $\tilde{\chi}(z)/(z - \omega)$ has no singularities within C ,

$$I_C = 0 \quad (8.80)$$

by Cauchy's integral theorem. The integral can be decomposed into

$$I_C = I_0 + I_r + I_R, \quad (8.81)$$

where

$$I_0 = \int_{-\infty}^{\omega-r} dz \frac{\tilde{\chi}(z)}{z - \omega} + \int_{\omega+r}^{\infty} dz \frac{\tilde{\chi}(z)}{z - \omega} \quad (8.82)$$

is evaluated on the real axis;

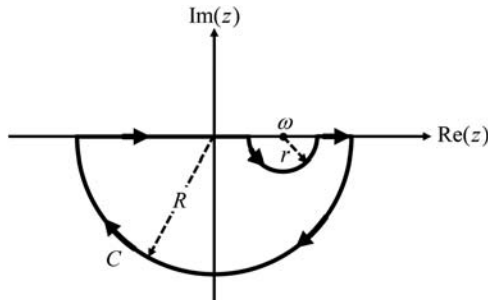


Figure 8.1 Integration path on the complex plane.

$$I_r = i \int_{-\pi}^0 d\theta \tilde{\chi}(\omega + re^{i\theta}) \quad (8.83)$$

is evaluated on the small circle $z - \omega = re^{i\theta} \Rightarrow dz = i re^{i\theta}$; and

$$I_R = \int_0^{-\pi} d\theta \frac{\tilde{\chi}(Re^{i\theta})}{Re^{i\theta} - \omega} i Re^{i\theta} \quad (8.84)$$

is evaluated on the large circle $z = Re^{i\theta} \Rightarrow dz = i Re^{i\theta}$.

Taking the limit $r \rightarrow 0$, we find that

$$\lim_{r \rightarrow 0} I_r = i\pi \tilde{\chi}(\omega), \quad (8.85)$$

$$\lim_{r \rightarrow 0} I_0 = \text{PV} \int_{-\infty}^{\infty} dz \frac{\tilde{\chi}(z)}{z - \omega}, \quad (8.86)$$

where PV denotes the principal value of the integral.

$\tilde{\chi}(\omega)$ is the dispersive part of the permittivity. As we noted in Section 8.4, $\lim_{\omega \rightarrow \infty} \tilde{\epsilon}(\omega) = 0$ on physical grounds. Assuming this to hold in the complex plane so that $\lim_{|z| \rightarrow \infty} \tilde{\chi}(z) = 0$, and that $\tilde{\chi}(\omega)$ falls off faster than $1/\omega$, we have

$$\lim_{R \rightarrow \infty} I_R = 0. \quad (8.87)$$

Thus, in the limits $r \rightarrow 0$ and $R \rightarrow \infty$, and from Eq. (8.88), we have

$$\begin{aligned} \lim_{\substack{R \rightarrow \infty \\ r \rightarrow 0}} I_C &= i\pi \tilde{\chi}(\omega) + \text{PV} \int_{-\infty}^{\infty} dz \frac{\tilde{\chi}(z)}{z - \omega} \\ &= 0. \end{aligned} \quad (8.88)$$

Thus,

$$\tilde{\chi}(\omega) = \frac{i}{\pi} \text{PV} \int_{-\infty}^{\infty} dz \frac{\tilde{\chi}(z)}{z - \omega}, \quad (8.89)$$

where z is now a real variable. Decomposing Eq. (8.89) into real and imaginary parts, and using $\tilde{\epsilon} = \tilde{\epsilon}_r + i\tilde{\epsilon}_i$, we have

$$\tilde{\epsilon}_r(\omega) + i\tilde{\epsilon}_i(\omega) = \epsilon_0 + \frac{i}{\pi} \text{PV} \int_{-\infty}^{\infty} dz \frac{\tilde{\epsilon}_r(z) + i\tilde{\epsilon}_i(z) - \epsilon_0}{z - \omega}. \quad (8.90)$$

Comparing the real and imaginary parts, we obtain the Kramers–Konig relations

$$\begin{aligned}
 \tilde{\epsilon}_r(\omega) &= \epsilon_0 - \frac{1}{\pi} \text{PV} \int_{-\infty}^{\infty} dz \frac{\tilde{\epsilon}_i(z)}{z - \omega} \\
 &= \epsilon_0 - \frac{2}{\pi} \text{PV} \int_0^{\infty} dz \frac{z \tilde{\epsilon}_i(z)}{z^2 - \omega^2},
 \end{aligned} \tag{8.91}$$

$$\begin{aligned}
 \tilde{\epsilon}_i(\omega) &= \frac{1}{\pi} \text{PV} \int_{-\infty}^{\infty} dz \frac{\tilde{\epsilon}_r(\omega) - \epsilon_0}{z - \omega} \\
 &= \frac{2\omega}{\pi} \text{PV} \int_0^{\infty} dz \frac{\tilde{\epsilon}_r(z)}{z^2 - \omega^2},
 \end{aligned} \tag{8.92}$$

where we have used the fact that

$$\text{PV} \int_0^{\infty} dz \frac{1}{z^2 - \omega^2} = 0. \tag{8.93}$$

Note 8.4

$$\begin{aligned}
 2\omega \text{PV} \int_0^{\infty} dz \frac{1}{z^2 - \omega^2} &= \lim_{\substack{L \rightarrow \infty \\ \delta \rightarrow 0}} \left(\int_0^{\omega-\delta} dz \frac{1}{z - \omega} + \int_{\omega+\delta}^L dz \frac{1}{z - \omega} - \int_0^R dz \frac{1}{z + \omega} \right) \\
 &= \lim_{\substack{L \rightarrow \infty \\ \delta \rightarrow 0}} [\log(-\delta) - \log(-\omega) + \log L - \log(\delta) - \log L + \log \omega] \\
 &= \lim_{\delta \rightarrow 0} [\log(-\delta) - \log(\delta) + \log \omega - \log(-\omega)] \\
 &= 0,
 \end{aligned} \tag{8.94}$$

using the fact that $-x = x e^{i\pi} \Rightarrow \log(-x) = \log x + i\pi$.

The Kramers–Kronig relations tell us that $\text{Re}(\tilde{\epsilon})$ and $\text{Im}(\tilde{\epsilon})$ are not independent and give formulae to calculate one from the other. An important physical consequence is that if $\tilde{\epsilon}_r(\omega) = \text{a constant}$, then Eqs. (8.92) and (8.93) imply that $\tilde{\epsilon}_i(\omega) = 0$. Hence, a nondispersive medium is nonconductive (non-absorbing), and a dispersive medium [$\tilde{\epsilon}_r(\omega) \neq \text{a constant}$] is conductive (absorbing), and $\tilde{\epsilon}_i(\omega) \neq 0$. Since metals are conductive, they are also dispersive.

In Section 8.2.2 we showed that when a material is conducting, its permittivity is $\epsilon_\omega = (\epsilon - i\sigma/\omega)$, which satisfies the Kramers–Kronig relation Eq. (8.91), but not Eq. (8.92). This is because the frequency-independent, real part of ϵ_ω , $\text{Re}(\epsilon_\omega)$, satisfies neither Eq. (8.61) nor the Kramers–Kronig relations.

Important Points of Chapter 8

- We write Maxwell's equations in a form suitable for computation. Computations can be cast into physical units by scaling.
- Linear nondispersive media don't exist but are a good model of reality within certain limitations.
- Maxwell's equations for linear media decompose into independent wave equations in $\mathbf{H}$ and $\mathbf{E}$ within uniform media but are coupled on media interfaces. Maxwell's equations imply wave equations, but not vice versa.
- We derive the dispersive form of Maxwell's equations.
- Conductivity implies dispersion.
- The Kramers–Kronig relations relate the real and imaginary parts of ϵ and are not independent.

Appendix 8.1 Properties of the Fourier Transform

A8.1.1 Definitions

The Fourier transform of a function $f(t)$ is defined by

$$\tilde{f}(\omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t} f(t), \quad (\text{A8.1.1})$$

where it is assumed that f is sufficiently “well-behaved” that the integral can be defined. Let $\mathbf{F}$ denote the Fourier transform operation; then $\tilde{f} = \mathbf{F}[f]$. The inverse Fourier transform $\mathbf{F}^{-1}$ is defined by $f = \mathbf{F}^{-1}[\tilde{f}]$, and

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \tilde{f}(\omega). \quad (\text{A8.1.2})$$

Note that the placement of the 2π factor differs according to author.

A8.1.2 Representation of the δ function

Inserting Eq. (A8.1.1) into Eq. (A8.1.2), we obtain

$$\begin{aligned} f(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \int_{-\infty}^{\infty} dt' e^{-i\omega t'} f(t') \\ &= \int_{-\infty}^{\infty} dt' f(t') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t')} \right]. \end{aligned} \quad (\text{A8.1.3})$$

The quantity $\Delta(t - t') \equiv (1/2\pi) \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t')}$ has the property [Eq. (A3.4.3)] of the δ function, $\delta(t - t')$ (see Appendix 3.4). For $t - t' \neq 0$, $\Delta(t - t') = 0$ because over an infinite range of frequencies, the frequency components of $\Delta(t - t')$ destructively interfere. Thus, $\Delta(t - t')$ has the property [Eq. (A3.4.1)]

of $\delta(t - t')$. Taking $f(t) = 1$, it is obvious that it also has the property of Eq. (A3.4.2). We therefore make the identification

$$\delta(t - t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t')}. \quad (\text{A8.1.4})$$

A8.1.3 Convolution theorem

Defining $\tilde{h}(\omega) = \tilde{f}(\omega)\tilde{g}(\omega)$, let us find $h = F^{-1}[\tilde{f}\tilde{g}]$. From Eq. (A8.1.2),

$$\begin{aligned} h(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \tilde{f}(\omega) \tilde{g}(\omega) \\ &= \int_{-\infty}^{\infty} dt' f(t') \int_{-\infty}^{\infty} dt'' g(t'') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega[(t-t')-t'']} \right] \\ &= \int_{-\infty}^{\infty} dt' f(t') \int_{-\infty}^{\infty} dt'' g(t'') \delta([t - t'] - t'') \\ &= \int_{-\infty}^{\infty} dt' f(t') g(t - t'), \end{aligned} \quad (\text{A8.1.5})$$

where the last equality is, by definition, the convolution of f and g . From this it is easy to show that

$$\begin{aligned} h(t) &= \int_{-\infty}^{\infty} dt' f(t') g(t - t') \\ &= \int_{-\infty}^{\infty} dt' g(t') f(t - t'). \end{aligned} \quad (\text{A8.1.6})$$

A8.1.4 Fourier transform of the derivative

Using definition Eq. (A8.1.1), let us evaluate $F[f']$, where $f'(t) = df(t)/dt$. By definition,

$$\begin{aligned} F[f'](\omega) &= \int_{-\infty}^{\infty} dt e^{-i\omega t} f'(t) \\ &= i\omega \int_{-\infty}^{\infty} dt e^{-i\omega t} f(t) + [e^{-i\omega t} f(t)] \Big|_{-\infty}^{\infty}, \end{aligned} \quad (\text{A8.1.7})$$

where the second equality is obtained from integration by parts. Physical quantities, such as electromagnetic fields, currents, and charge densities, are localized in space and time, so they vanish at infinity. Assuming f to be such a physical quantity, we are left with

$$F[f'](\omega) = i\omega\tilde{f}(\omega). \quad (\text{A8.1.8})$$

Thus, $\partial_t f(t)$ in the time domain is equivalent to $i\omega\tilde{f}(\omega)$ in the frequency domain.

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Chapter 9

The Yee Algorithm in One Dimension

The Yee algorithm¹ is *one* realization (others are possible) of the FDTD methodology to solve Maxwell's equations based on second-order central finite differences. In this chapter we develop the Yee algorithm for a linear nondispersive medium. Following our strategy of stepwise increasing complexity, we develop the Yee algorithm in one dimension to avoid the distracting technical details that arise in two and three. Nonetheless, there are many 'devils in the details.'

9.1 Basic Solution of Maxwell's Equations

Maxwell's equations in one dimension might seem trivial, uninteresting, and of little practical use, but in fact we gain some interesting insights by examining them.

Maxwell's equations in a linear nonconducting medium are

$$\mu \partial_t \mathbf{H} = -\nabla \times \mathbf{E}, \quad (9.1a)$$

$$\epsilon \partial_t \mathbf{E} = \nabla \times \mathbf{H}. \quad (9.1b)$$

Taking $H_x = H_y = 0$ and $H_z = H_z(x, t)$, and $E_x = E_z = 0$ and $E_y = E_y(x, t)$ (which implies that $\partial_y H_z = \partial_z H_z = 0$, $\partial_y E_y = \partial_z E_y = 0$), in one dimension Maxwell's equations reduce to

$$\mu \partial_t H_z = -\partial_x E_y, \quad (9.2a)$$

$$\epsilon \partial_t E_y = -\partial_x H_z. \quad (9.2b)$$

This describes an electromagnetic field with $\mathbf{E}$ polarized along the y axis.

Alternatively, one could take $H_x = H_z = 0$ and $H_y = H_y(x, t)$, and $E_x = E_y = 0$ and $E_z = E_z(x, t)$, in which case Maxwell's equations reduce to

$$\mu \partial_t H_y = \partial_x E_z, \quad (9.3a)$$

$$\varepsilon \partial_t E_z = \partial_x H_y. \quad (9.3b)$$

In this case, $\mathbf{E}$ is polarized along the z axis.

When ε and μ are space-time invariant, both of the above sets of Maxwell's equations [Eqs. (9.2) and (9.3)] reduce to the wave equation,

$$\left(\partial_t^2 - \frac{1}{\varepsilon \mu} \partial_x^2 \right) (H, E) = 0, \quad (9.4)$$

where $(H, E) = (H_z, E_y)$ or (H_y, E_z) . However, the wave equation and Maxwell's equations are not equivalent. While the wave equation is invariant under the transformation $(\varepsilon, \mu) \rightarrow -(\varepsilon, \mu)$, Maxwell's equations are not. It is for this reason that metamaterials, in which both ε and μ are negative, have very different properties from ordinary materials.

Because $\mathbf{H}$ and $\mathbf{E}$ separate in the derivation of Eq. (9.4), the wave equation gives no information about their relationship. Solutions of Eq. (9.4) propagating in the $\pm x$ directions are $H(x, t) = f_H(x \mp vt)$ and $E(x, t) = f_E(x \mp vt)$, where f_H and f_E are arbitrary independent functions, and $v = \sqrt{1/\varepsilon \mu}$. On the other hand, by direct substitution it can be shown that solutions of Eqs. (9.2) and (9.3) propagating in the $\pm x$ direction are, respectively,

$$E_y(x, t) = f(x \mp vt), \quad (9.5a)$$

$$H_z(x, t) = \pm \sqrt{\frac{\varepsilon}{\mu}} E_y(x, t), \quad (9.5b)$$

and

$$E_z(x, t) = f(x \mp vt), \quad (9.6a)$$

$$H_y(x, t) = \mp \sqrt{\frac{\varepsilon}{\mu}} E_z(x, t). \quad (9.6b)$$

9.2 Standard Yee Algorithm

9.2.1 Zero conductivity

Let us now proceed to set up an FDTD algorithm to solve the 1D Maxwell equations given by Eq. (9.3). Replacing the derivatives with central finite-difference approximations, we obtain the standard finite difference (S-FD) model,

$$\mu(x) \frac{d_t H_y(x, t)}{d_x} = \frac{\Delta t}{\Delta x} d_x E_z(x, t), \quad (9.7a)$$

$$\varepsilon(x) \frac{d_t E_z(x, t)}{d_x} = \frac{\Delta t}{\Delta x} d_x H_y(x, t). \quad (9.7b)$$

For notational brevity, let us define

$$E_z|_\chi^\tau = E_z(\chi \Delta x, \tau \Delta t), \quad (9.8a)$$

$$H_y|_\chi^\tau = H_y(\chi \Delta x, \tau \Delta t), \quad (9.8b)$$

$$\mu_\chi = \mu(\chi \Delta x), \quad (9.8c)$$

$$\varepsilon_\chi = \varepsilon(\chi \Delta x), \quad (9.8d)$$

where $\chi = 0, 1, 2, \dots, N$, and $\tau = 0, 1, 2, \dots$. With these definitions,

$$\begin{aligned} d_t F(\chi \Delta x, \tau \Delta t) &= F|_\chi^{\tau+1/2} - F|_\chi^{\tau-1/2} \\ &= d_\tau F|_\chi^\tau, \end{aligned} \quad (9.9a)$$

and

$$\begin{aligned} d_x F(\chi \Delta x, \tau \Delta t) &= F|_{\chi+1/2}^\tau - F|_{\chi-1/2}^\tau \\ &= d_\chi F|_\chi^\tau, \end{aligned} \quad (9.9b)$$

where $F = E_z$ or H_y . Model Eq. (9.7) now becomes

$$d_\tau H_y|_\chi^\tau = \frac{\Delta t}{\mu_\chi \Delta x} d_\chi E_z|_\chi^\tau, \quad (9.10a)$$

$$d_\tau E_z|_\chi^\tau = d_\chi H_y|_\chi^\tau. \quad (9.10b)$$

Expanding the difference operators and solving for $H_y|_\chi^{\tau+1/2}$ and $E_z|_\chi^{\tau+1/2}$, we obtain

$$H_y|_\chi^{\tau+1/2} = H_y|_\chi^{\tau-1/2} + \frac{\Delta t}{\mu_\chi \Delta x} \left(E_z|_{\chi+1/2}^\tau - E_z|_{\chi-1/2}^\tau \right), \quad (9.11a)$$

$$E_z|_\chi^{\tau+1/2} = E_z|_\chi^{\tau-1/2} + \frac{\Delta t}{\varepsilon_\chi \Delta x} \left(H_y|_{\chi+1/2}^\tau - H_y|_{\chi-1/2}^\tau \right). \quad (9.11b)$$

Unfortunately, this algorithm cannot be iterated because it requires field values between the space–time grid points $(\chi \Delta x, \tau \Delta t)$. This difficulty can be circumvented by modeling $\mathbf{H}$ and $\mathbf{E}$ at different space–time grid points.

For example, we could take E_z to lie on $(\chi \Delta x, \tau \Delta t)$ and H_y to lie in between on $[(\chi + \frac{1}{2})\Delta x]$, $[(\tau \pm \frac{1}{2})\Delta t]$, as shown in Fig. 9.1. Model Eq. (9.10) now becomes what we call the **standard Yee model**:

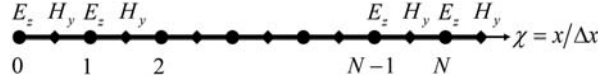


Figure 9.1 A possible layout of the electric and magnetic fields on the spatial grid for the Yee algorithm.

$$d_\tau H_y|_{\chi+1/2}^\tau = \frac{\Delta t}{\Delta x} \frac{1}{\mu_{\chi+1/2}} d_\chi E_z|_{\chi+1/2}^\tau, \quad (9.12a)$$

$$d_\tau E_z|_\chi^{\tau+1/2} = \frac{\Delta t}{\Delta x} \frac{1}{\epsilon_\chi} d_\chi H_y|_{\chi+1/2}^{\tau+1/2}, \quad (9.12b)$$

from which we obtain the **standard Yee algorithm**:

$$\begin{aligned} H_y|_{\chi+1/2}^{\tau+1/2} &= H_y|_{\chi+1/2}^{\tau-1/2} + \frac{\Delta t}{\Delta x} \frac{1}{\mu_{\chi+1/2}} d_\chi E_z|_{\chi+1/2}^\tau \\ &= H_y|_{\chi+1/2}^{\tau-1/2} + \frac{\Delta t}{\Delta x} \frac{1}{\mu_{\chi+1/2}} (E_z|_{\chi+1}^\tau - E_z|_\chi^\tau) \end{aligned} \quad (9.13a)$$

for $0 \leq \chi \leq N-1$, and

$$\begin{aligned} E_z|_\chi^{\tau+1} &= E_z|_\chi^\tau + \frac{\Delta t}{\Delta x} \frac{1}{\epsilon_\chi} d_\chi H_y|_{\chi+1/2}^{\tau+1/2} \\ &= E_z|_\chi^\tau + \frac{\Delta t}{\Delta x} \frac{1}{\epsilon_\chi} (H_y|_{\chi+1/2}^{\tau+1/2} - H_y|_{\chi-1/2}^{\tau+1/2}) \end{aligned} \quad (9.13b)$$

for $1 \leq \chi \leq N$.

Notice that neither $H_y|_{N+1/2}^{\tau+1/2}$ nor $E_z|_0^{\tau+1/2}$ on the boundary of the computational domain can be computed using the Yee algorithm. They must be computed separately, as discussed in Section 9.3. Notice that $\mathbf{H}$ and $\mathbf{E}$ are computed at different positions and also that ϵ and μ are specified at different positions. Given the initial fields $H_y|_{\chi+1/2}^{-1/2}$ and $E_z|_\chi^0$ ($\chi=0,1,\dots,N$), Eq. (9.13) can be iterated.

The Yee algorithm—hereafter referred to as the S (standard) Yee algorithm—is implemented in pseudocode in Appendix 9.2 and in Program MC9.1.

9.2.2 Including conductivity

When a conduction current is included, Maxwell's equations become

$$\mu \partial_t H_y = \partial_x E_z, \quad (9.14a)$$

$$\epsilon \partial_t E_z = \partial_x H_y - \sigma E_z. \quad (9.14b)$$

It is straightforward to derive the **standard Yee model with conductivity**:

$$d_\tau H_y|_{\chi+1/2}^\tau = \frac{\Delta t}{\Delta x} \frac{1}{\mu_{\chi+1/2}} d_\chi E_z|_{\chi+1/2}^\tau, \quad (9.15a)$$

$$d_\tau E_z|_\chi^{\tau+1/2} = \frac{\Delta t}{\Delta x} \frac{1}{\varepsilon_\chi} d_\chi H_y|_{\chi+1/2}^{\tau+1/2} - \frac{\sigma_\chi \Delta t}{\varepsilon_\chi} E_z|_\chi^{\tau+1/2}. \quad (9.15b)$$

Conductivity complicates the implementation of the Yee model [Eq. (9.15)] into an algorithm that can be iterated. Since E_z is evaluated at time $t + \Delta t/2$, the quantities on the right side must also be evaluated at the same time; however, because $E_z|_\chi^{\tau+1/2}$ is not computed, it must be approximated. There are three possible choices:

$$E_z|_\chi^{\tau+1/2} \cong E_z|_\chi^{\tau+1}, \quad (9.16a)$$

$$E_z|_\chi^{\tau+1/2} \cong E_z|_\chi^\tau, \quad (9.16b)$$

$$E_z|_\chi^{\tau+1/2} \cong \frac{1}{2} \left(E_z|_\chi^{\tau+1} + E_z|_\chi^\tau \right). \quad (9.16c)$$

Assuming a uniform region in which both ε and μ are constant, and using choice Eq. (9.16c), Eq. (9.15b) becomes

$$\varepsilon d_\tau E_z|_\chi^{\tau+1/2} = \frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2} - \frac{1}{2} \sigma \Delta t \left(E_z|_\chi^{\tau+1} + E_z|_\chi^\tau \right). \quad (9.17)$$

Multiplying both sides of Eq. (9.17) by μ , applying d_τ , and employing Eq. (9.15a) in the form

$$\mu d_\tau H_y|_\chi^{\tau+1/2} = \frac{\Delta t}{\Delta x} d_\chi E_z|_\chi^{\tau+1/2}, \quad (9.18)$$

we obtain

$$\varepsilon \mu d_\tau^2 E_z|_\chi^{\tau+1/2} = \frac{\Delta t^2}{\Delta x^2} d_\chi^2 E_z|_\chi^{\tau+1/2} - \frac{1}{2} \mu \sigma \Delta t \left(d_\tau E_z|_\chi^{\tau+1} + d_\tau E_z|_\chi^\tau \right), \quad (9.19)$$

where $d_\tau^2 = d_\tau d_\tau$, and $d_\chi^2 = d_\chi d_\chi$. Using $d_\tau E_z|_\chi^{\tau+1} + d_\tau E_z|_\chi^\tau = E_z|_\chi^{\tau+3/2} - E_z|_\chi^{\tau-1/2}$, and making the shift $\tau \rightarrow \tau - 1/2$, Eq. (9.19) becomes

$$d_\tau^2 E_z|_\chi^\tau = \frac{1}{\varepsilon \mu} \frac{\Delta t}{\Delta x} d_\chi^2 E_z|_\chi^\tau - \frac{\sigma \Delta t}{2\varepsilon} \left(E_z|_\chi^{\tau+1} - E_z|_\chi^{\tau-1} \right). \quad (9.20)$$

Setting $\alpha = \sigma/2\varepsilon$ and $\nu^2 = 1/\varepsilon\mu$ in Eq. (9.20), we obtain

$$d_\tau^2 E_z|_\chi^\tau + \alpha \Delta t (E_z|_\chi^{\tau+1} - E_z|_\chi^{\tau-1}) + \frac{\nu^2 \Delta t^2}{\Delta x^2} d_\chi^2 E_z|_\chi^\tau = 0, \quad (9.21)$$

which is simply the SC (standard central) FD model of the damped wave equation given in Eq. (5.20).

Thus, $E_z|_\chi^{\tau+1/2} \cong (E_z|_\chi^{\tau+1} + E_z|_\chi^\tau)/2$ in the S-Yee model is equivalent to the SC-FD model of the damped wave equation. Similarly, it can be shown that the choices of Eqs. (9.16a) and (9.16b) are equivalent to the S-forward and S-backward FD models of the damped wave equation, respectively.

In Section 5.2.2 we showed that the SC-FD model of the damped wave equation is the most accurate, so we choose Eq. (9.16c) to model Maxwell's conducting equations. Thus, the FD model becomes

$$\varepsilon_\chi d_\tau E_z|_\chi^{\tau+1/2} = \frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2} - \frac{1}{2} \sigma_\chi \Delta t (E_z|_\chi^{\tau+1} + E_z|_\chi^\tau), \quad (9.22)$$

which is equivalent to

$$d_\tau E_z|_\chi^{\tau+1/2} = \frac{1}{\varepsilon_\chi} \frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2} - \frac{\sigma_\chi \Delta t}{2\varepsilon_\chi} (E_z|_\chi^{\tau+1} + E_z|_\chi^\tau). \quad (9.23)$$

Expanding the difference expressions and solving for $E_z|_\chi^{\tau+1}$, we obtain

$$E_z|_\chi^{\tau+1} = \frac{1}{(1 + \sigma_\chi \Delta t/2\varepsilon_\chi)} \left[(1 - \sigma_\chi \Delta t/2\varepsilon_\chi) E_z|_\chi^\tau + \frac{\Delta t}{\Delta x} \frac{1}{\varepsilon_\chi} d_\chi H_y|_\chi^{\tau+1/2} \right], \quad (9.24)$$

which, together with Eq. (9.13a), constitutes the Yee algorithm with linear conductivity.

9.2.3 Including source current and conductivity

Finally, let us incorporate a source current into the Yee algorithm. Taking $J_{s,z} = J_{s,z}(x, t)$ and $J_{s,x} = J_{s,y} = 0$, Maxwell's equations become

$$\mu \partial_t H_y = \partial_x E_z, \quad (9.25a)$$

$$\varepsilon \partial_t E_z = \partial_x H_y - \sigma E_z - J_{s,z}. \quad (9.25b)$$

Including a source current in model Eq. (9.22), the Yee model of Eq. (9.25b) is

$$E_z|_\chi^{\tau+1} (\varepsilon_\chi + \sigma_\chi/2) - E_z|_\chi^\tau (\varepsilon_\chi - \sigma_\chi/2) = \frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2} - \Delta t J_{s,z}|_\chi^{\tau+1/2}. \quad (9.26)$$

Thus, we obtain the **Yee algorithm including source current and conductivity**:

$$H_y|_{\chi+1/2}^{\tau+1/2} = H_y|_{\chi+1/2}^{\tau-1/2} + \frac{\Delta t}{\Delta x} \frac{1}{\mu_{\chi+1/2}} d_\chi E_z|_{\chi+1/2}^\tau \quad \text{for } 0 \leq \chi \leq N-1, \quad (9.27a)$$

$$E_z|_\chi^{\tau+1} = \frac{1}{(1 + \sigma_\chi \Delta t / 2\epsilon_\chi)} \left\{ (1 - \sigma_\chi \Delta t / 2\epsilon_\chi) E_z|_\chi^\tau + \frac{1}{\epsilon_\chi} \left[\frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2} - \Delta t J_{s,z}|_\chi^{\tau+1/2} \right] \right\} \quad (9.27b)$$

for $1 \leq \chi \leq N$.

If there is no initial electromagnetic field [$H_y(x, t) = 0$ for $t \leq -\Delta t/2$ and $E_z(x, t) = 0$ for $t \leq 0$] and the source current turns on at $t = 0$ [$J_z(x, t) = 0$ for $t \leq 0$], then taking the initial fields to be $H_y|_{\chi+1/2}^{-1/2} = 0$ and $E_z|_\chi^0 = 0$ ($\chi = 0, 1, \dots, N$), we can iterate the Yee algorithm of Eq. (9.27).

For example, let $J_{s,z}(x, t)$ be a point source of the form

$$J_{s,z}(x, t) = \delta(x)j(t), \quad (9.28)$$

where $j(t) = 0$ for $t \leq 0$. Modeling $\delta(x)$ by $\delta_{x,0}/\Delta x$, in a nonconducting medium uniform with $\epsilon = 1$, the **Yee algorithm with a point source current in a uniform nonconducting medium** is

$$H_y|_{\chi+1/2}^{\tau+1/2} = H_y|_{\chi+1/2}^{\tau-1/2} + \frac{\Delta t}{\Delta x} \frac{1}{\mu} d_\chi E_z|_{\chi+1/2}^\tau \quad \text{for } 0 \leq \chi \leq N-1, \quad (9.29a)$$

$$E_z|_\chi^{\tau+1} = E_z|_\chi^\tau + \frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2} - \frac{\Delta t}{\Delta x} \delta_{x,0} j|_\chi^{\tau+1/2} \quad \text{for } 1 \leq \chi \leq N, \quad (9.29b)$$

where μ is constant. The analytic solution for the electromagnetic field due to this source current is derived in Appendix 9.1.

9.2.4 Alternative configurations of the Yee algorithm

In Eq. (9.13) H_y is evaluated at $t = (\tau + 1/2)\Delta t$ and $x = (\chi + 1/2)\Delta x$, but it could also be evaluated at $x = (\chi - 1/2)\Delta x$ at the same t values, as shown in Fig. 9.2.

In this case, the Yee algorithm becomes

$$H_y|_{\chi-1/2}^{\tau+1/2} = H_y|_{\chi-1/2}^{\tau-1/2} + \frac{\Delta t}{\Delta x} \frac{1}{\mu_{\chi-1/2}} (E_z|_\chi^\tau - E_z|_{\chi-1}^\tau) \quad \text{for } 1 \leq \chi \leq N, \quad (9.30a)$$

$$E_z|_\chi^{\tau+1} = E_z|_\chi^\tau + \frac{\Delta t}{\Delta x} \frac{1}{\epsilon_\chi} (H_y|_{\chi+1/2}^{\tau+1/2} - H_y|_{\chi-1/2}^{\tau+1/2}) \quad \text{for } 0 \leq \chi \leq N-1. \quad (9.30b)$$

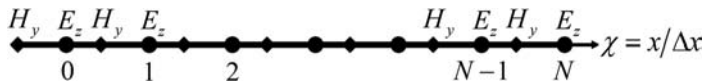


Figure 9.2 Alternative layout of the electric and magnetic fields on the spatial grid for the Yee algorithm.

Now $H_y|_{-1/2}^{\tau+1/2}$ and $E_z|_N^{\tau+1}$ lie on the computational boundary and must be computed separately. Algorithm Eq. (9.30) is implemented in Program MC9.2.

It is also possible to update E_z first, and then H_y ; and the position of E_z relative to H_y can be changed.

9.3 Computational Boundaries

The field values on the computational boundary cannot be calculated with the Yee algorithm. In Eq. (9.25b), $H_y|_{N+1/2}^{\tau+1/2}$ is needed to compute $E_z|_N^{\tau+1}$, but Eq. (9.25a) gives no prescription for computing it; similarly, Eq. (9.25a) requires the value of $E_z|_0^\tau$, but it is not computed in Eq. (9.25b). Following Section 6.1, a reflecting, periodic, or absorbing boundary condition (ABC) can be defined. A reflecting boundary is given by

$$H_y|_{N+1/2}^{\tau+1/2} = E_z|_0^{\tau+1} = 0, \quad (9.31)$$

and a periodic boundary is given by

$$H_y|_{N+1/2}^{\tau+1/2} = H_y|_0^{\tau+1/2}, \quad (9.32a)$$

$$E_z|_0^{\tau+1} = E_z|_N^{\tau+1}. \quad (9.32b)$$

Assuming the medium on the boundary grid points one spacing inside to be uniform, both H_y and E_z obey the wave equation, so we can use the ABC developed in Section 6.1.3. From Eq. (6.21) we obtain

$$H_y|_{N+1/2}^{\tau+1/2} = H_y|_{N-1/2}^{\tau-1/2} + \left(\frac{1-u}{1+u} \right) \left(H_y|_{N+1/2}^{\tau-1/2} - H_y|_{N-1/2}^{\tau+1/2} \right), \quad (9.33a)$$

where $u = \nu \Delta t / \Delta x$, and from Eq. (6.24),

$$E_z|_0^{\tau+1} = E_z|_1^\tau - \left(\frac{1-u}{1+u} \right) \left(E_z|_1^{\tau+1} - E_z|_0^\tau \right). \quad (9.33b)$$

When $u = 1$, this approximate ABC reduces to the perfect ABC given by

$$H_y|_{N+1/2}^{\tau+1/2} = H_y|_{N-1/2}^{\tau-1/2}, \quad (9.34a)$$

$$E_z|_0^{\tau+1} = E_z|_1^\tau. \quad (9.34b)$$

Algorithm Eq. (9.13) together with computational boundary conditions are implemented in Program MC9.1 and in pseudocode in Appendix 9.2.

9.4 The Nonstandard Yee Algorithm

9.4.1 Zero conductivity

To develop the nonstandard (NS) Yee algorithm, it is convenient to define

$$B'_y = \frac{\Delta x}{\Delta t} \mu H_y, \quad (9.35)$$

where $B_y = \mu H_y$. The S-FD model of Eq. (9.7) becomes

$$d_t B'_y(x, t) = d_x E_z(x, t), \quad (9.36a)$$

$$d_t E_z(x, t) = \frac{1}{\varepsilon \mu} \frac{\Delta t^2}{\Delta x^2} d_x B'_y(x, t). \quad (9.36b)$$

In each region of constant $v = 1/\sqrt{\varepsilon \mu}$, Eq. (9.36) yields two S-FD wave equation models:

$$\left(d_t^2 - \frac{v^2 \Delta t^2}{\Delta x^2} d_x^2 \right) (H_y, E_z) = 0. \quad (9.37)$$

Following the development of the NS-FD model for the wave equation in Section 4.2.3, we put

$$\frac{v \Delta t}{\Delta x} \rightarrow \tilde{v} = \frac{\sin(\omega \Delta t/2)}{\sin(k \Delta x/2)}, \quad (9.38)$$

where k is the wavenumber, and $\omega = vk$. What we now call the NS-Yee model of Maxwell's equations is

$$d_\tau B'_y|_{\chi+1/2}^\tau = d_\chi E_z|_{\chi+1/2}^\tau, \quad (9.39a)$$

$$d_\tau E_z|_\chi^{\tau+1/2} = \tilde{v}_\chi^2 d_\chi B'_y|_\chi^{\tau+1/2}, \quad (9.39b)$$

and the NS-Yee algorithm becomes

$$B'_y|_{\chi+1/2}^{\tau+1/2} = B'_y|_{\chi+1/2}^{\tau-1/2} + d_\chi E_z|_{\chi+1/2}^\tau \quad \text{for } 0 \leq \chi \leq N-1, \quad (9.40a)$$

$$E_z|_\chi^{\tau+1} = E_z|_\chi^\tau + \tilde{v}_\chi^2 d_\chi B'_y|_\chi^{\tau+1/2} \quad \text{for } 1 \leq \chi \leq N. \quad (9.40b)$$

Given $B'_y|_{\chi+1/2}^{-1/2}$ and $E_z|_\chi^0$, this algorithm can be iterated for $\chi = 0, 1, \dots, N$.

Devil in the details

The Yee realization of Eq. (9.36b) is

$$d_\tau E_z|_\chi^{\tau+1/2} = \frac{1}{\epsilon_\chi \mu_\chi} \frac{\Delta t^2}{\Delta x^2} d_\chi B_y|_\chi^{\tau+1/2}, \quad (9.41)$$

which we want to be equivalent to

$$d_\tau E_z|_\chi^{\tau+1/2} = \frac{1}{\epsilon_\chi} \frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2}. \quad (9.42)$$

But in Eq. (9.40a) B_y' is computed at $x = (\chi + 1/2)h$, so μ must also be specified at $x = (\chi + 1/2)h$. Thus,

$$\begin{aligned} H_y|_{\chi+1/2}^{\tau+1/2} - H_y|_{\chi-1/2}^{\tau+1/2} &= \frac{1}{\mu_{\chi+1/2}} B_y'|_{\chi+1/2}^{\tau+1/2} - \frac{1}{\mu_{\chi-1/2}} B_y'|_{\chi-1/2}^{\tau+1/2} \\ &\neq \frac{1}{\mu_\chi} \frac{\Delta t}{\Delta x} \left(B_y'|_{\chi+1/2}^{\tau+1/2} - B_y'|_{\chi-1/2}^{\tau+1/2} \right). \end{aligned} \quad (9.43)$$

If, however, the variation of μ is small over a wavelength, then it is a reasonable approximation to take

$$d_\chi H_y|_\chi^{\tau+1/2} = \frac{1}{\mu_\chi} \frac{\Delta t}{\Delta x} d_\chi B_y|_\chi^{\tau+1/2}. \quad (9.44)$$

9.4.2 Including conductivity

The standard Yee model with conductivity is

$$d_\tau E_z|_\chi^{\tau+1/2} = \frac{1}{\epsilon_\chi} \frac{\Delta t}{\Delta x} d_\chi H_y|_\chi^{\tau+1/2} - \frac{\sigma_\chi \Delta t}{2\epsilon_\chi} \left(E_z|_\chi^{\tau+1} + E_z|_\chi^\tau \right). \quad (9.45)$$

Rewriting this model in terms of B_y' via Eq. (9.35), we obtain

$$d_\tau E_z|_\chi^{\tau+1/2} = \frac{1}{\epsilon_\chi \mu_\chi} \frac{\Delta t^2}{\Delta x^2} d_\chi B_y'|_\chi^{\tau+1/2} - \frac{\sigma_\chi \Delta t}{2\epsilon_\chi} \left(E_z|_\chi^{\tau+1} + E_z|_\chi^\tau \right). \quad (9.46)$$

Following the development that led to Eqs. (9.20) and (9.21), we obtain an FD model of the absorbing wave equation. The exact NS-FD model is given by Eq. (5.31), and with the substitutions $\sigma/2\epsilon \rightarrow \tilde{\alpha}'$ and $1/\epsilon\mu \rightarrow \tilde{\nu}'^2$, we obtain an exact NS-FD model of the conducting Maxwell's equations,

$$B_y'|_{\chi+1/2}^{\tau+1/2} = B_y'|_{\chi+1/2}^{\tau-1/2} + d_\chi E_z|_{\chi+1/2}^\tau, \quad (9.47a)$$

$$d_\tau E_z|_\chi^{\tau+1/2} = \tilde{\nu}'^2 d_\chi H_y|_\chi^{\tau+1/2} - \tilde{\alpha}' \left(E_z|_\chi^{\tau+1} + E_z|_\chi^\tau \right), \quad (9.47b)$$

where

$$\tilde{v}^2 = \frac{2 \sin^2(\omega \Delta t/2)}{1 - \cos(k'_r \Delta x) \cosh(k'_i \Delta x)}, \quad (9.48a)$$

$$\tilde{\alpha}' = -\tan(\omega \Delta t/2) \frac{\sin(k'_r \Delta x) \sinh(k'_i \Delta x)}{1 - \cos(k'_r \Delta x) \cosh(k'_i \Delta x)}, \quad (9.48b)$$

and $k' = k'_r + i k'_i$ is given by Eq. (4.49). With $\alpha = \sigma/2\varepsilon$,

$$k' = \frac{k}{\sqrt{2\omega}} \left[\left(\sqrt{\omega^2 + \sigma^2/\varepsilon^2} + \omega \right)^{1/2} - i \left(\sqrt{\omega^2 + \sigma^2/\varepsilon^2} - \omega \right)^{1/2} \right]. \quad (9.49)$$

The NS-Yee algorithm with conductivity is thus

$$B'_y|_{\chi+1/2}^{\tau+1/2} = B'_y|_{\chi+1/2}^{\tau-1/2} + d_\chi E_z|_{\chi+1/2}^\tau \quad \text{for } 0 \leq \chi \leq N-1, \quad (9.50a)$$

$$E_z|_\chi^{\tau+1} = \frac{1}{1+\tilde{\alpha}'_\chi} \left[(1 - \tilde{\alpha}'_\chi) E_z|_\chi^\tau + \tilde{v}_\chi^2 d_\chi B'_y|_\chi^{\tau+1/2} \right] \quad \text{for } 1 \leq \chi \leq N, \quad (9.50b)$$

where $\tilde{\alpha}'_\chi$ is computed using the local value of k' , that is, k'_χ .

9.4.3 Including a source current

When the electromagnetic field is generated by a source current, the NS-FD model of Maxwell's equations (zero conductivity) becomes

$$d_t B'_y(x, t) = d_x E_z(x, t), \quad (9.51a)$$

$$d_t E_z(x, t) = \tilde{v}^2 d_x B'_y(x, t) - \tilde{J}_{s,z}(x, t), \quad (9.51b)$$

where $\tilde{J}_{s,z}$ is the NS model of the source current. Notice that the factor of $\Delta t/\varepsilon$, which appears in the S-Yee algorithm [Eq. (9.27b)] for $\sigma=0$, is subsumed into $\tilde{J}_{s,z}$.

The NS model for $J_{s,z}$ depends on its functional form. To determine $\tilde{J}_{s,z}$, it is convenient to cast the NS-FD model of Maxwell's equations [Eq. (9.51)] into a pair of inhomogeneous wave equation models. It is easy to show that these are

$$(d_t^2 - \tilde{v}^2 d_x^2) B'_y(x, t) = -d_x \tilde{J}_{s,z}(x, t), \quad (9.52a)$$

$$(d_t^2 - \tilde{v}^2 d_x^2) E_z(x, t) = -d_t \tilde{J}_{s,z}(x, t). \quad (9.52b)$$

Point source current

For example, let

$$J_{s,z} = \delta(x) \Theta(t) e^{i\omega t}, \quad (9.53)$$

and postulate that

$$\tilde{J}_{s,z} = \tilde{A} \delta_{x,0} \Theta(t) e^{i\omega t}, \quad (9.54)$$

where the factor $\tilde{A}$ is to be determined.

The analytic solution for the electromagnetic field produced by the source current of Eq. (9.53) is

$$H_y(x,t) = \frac{1}{2} \text{sgn}(x) \Theta(t - |x|/\nu) e^{i(\omega t - k|x|)}, \quad (9.55)$$

$$E_z(x,t) = -\frac{1}{2\nu} \Theta(t - |x|/\nu) e^{i(\omega t - k|x|)}, \quad (9.56)$$

as shown in Appendix 9.1. Inserting Eq. (9.56) into Eq. (9.52b) at $x=0$ for $t > \Delta x/\nu$, and using the identities

$$\frac{d_t e^{i\omega t}}{e^{i\omega t}} = 2i \sin(\omega \Delta t/2), \quad (9.57a)$$

$$\frac{d_t^2 e^{i\omega t}}{e^{i\omega t}} = -4 \sin^2(\omega \Delta t/2), \quad (9.57b)$$

$$d_x^2 e^{-ik|x|}|_{x=0} = -4i e^{-ik\Delta x/2} \sin(k\Delta x/2), \quad (9.57c)$$

and the relationship $\sin(\omega \Delta t/2) = \tilde{\nu} \sin(k\Delta x/2)$, we obtain

$$\frac{\tilde{\nu}}{\nu} \left[-\sin(k\Delta x/2) + i e^{-ik\Delta x/2} \right] = i \tilde{A} \quad (9.58)$$

and find that

$$\begin{aligned} \tilde{A} &= \frac{\sin(\omega \Delta t/2)}{\nu \tan(k\Delta x/2)} \\ &= \frac{k \sin(\omega \Delta t/2)}{\omega \tan(k\Delta x/2)}. \end{aligned} \quad (9.59)$$

It can be verified that the same result is obtained when the analytic solution for H_y [Eq. (9.55)] is inserted into Eq. (9.52a) with the substitution $\nu \Delta t/\Delta x \rightarrow \tilde{\nu}$ in conjunction with $\mu = 1/\nu^2$. Compare with NS amplitude given by Eq. (5.51) for the wave equation.

The NS-Yee algorithm for a harmonic point source current of angular frequency ω located at position $x = p\Delta x$ is thus

$$B'_y|_{\chi+1/2}^{\tau+1/2} = B'_y|_{\chi+1/2}^{\tau-1/2} + d_\chi E_z|_{\chi+1/2}^{\tau+1/2} \quad \text{for } 0 \leq \chi \leq N-1, \quad (9.60a)$$

$$E_z|_{\chi}^{\tau+1} = E_z|_{\chi}^{\tau} + \tilde{v}_\chi^2 d_\chi B'_y|_{\chi}^{\tau+1/2} - \tilde{A} \delta_{\chi,p} j_\omega|_{\chi+1/2}^{\tau+1/2} \quad \text{for } 1 \leq \chi \leq N, \quad (9.60b)$$

where $j_\omega(t) = 0$ for $t \leq 0$ is a harmonic function of angular frequency ω . Assuming no initial electromagnetic field, this algorithm can be iterated with the initial conditions $B'_y|_{\chi+1/2}^{-1/2} = 0$ and $E_z|_{\chi}^0 = 0$ for $\chi = 0, 1, \dots, N$.

In most FDTD calculations, the electromagnetic fields are generated in free space (or within a uniform nonconducting substrate) and then propagated onto a structure of interest. We therefore omit the case of a source within a conducting dielectric.

Constant magnetic permeability

Except in ferromagnetic materials, the magnetic permeability is often constant and close and to its free-space value, and $\mu \approx \mu_0$ even across dielectric interfaces; in our unit system (see Chapter 6), $\mu_0 = 1/c^2$. Thus, while ϵ varies with the material, it is often a good approximation to take μ everywhere to be constant.

Let $\epsilon = 1$ in medium 1 in which the electromagnetic propagation velocity is $v_0 = 1/\sqrt{\mu}$; let medium 2 have the same μ but different ϵ , with $v = v_0/\sqrt{\epsilon}$ and index refraction $n = \sqrt{\epsilon}$. Following the development of the NS-FD model of the wave equation, the NS-Yee algorithm [Eq. (9.40)] becomes

$$B'_y|_{\chi+1/2}^{\tau+1/2} = B'_y|_{\chi+1/2}^{\tau-1/2} + d_\chi E_z|_{\chi+1/2}^{\tau+1/2} \quad \text{for } 0 \leq \chi \leq N-1, \quad (9.61a)$$

$$E_z|_{\chi}^{\tau+1} = E_z|_{\chi}^{\tau} + \frac{\tilde{v}_0^2}{\tilde{\epsilon}_\chi} d_\chi B'_y|_{\chi}^{\tau+1/2} - \tilde{J}_{s,z}|_{\chi}^{\tau+1/2} \quad \text{for } 1 \leq \chi \leq N, \quad (9.61b)$$

where $\tilde{\epsilon} = \tilde{n}^2$, as given by Eq. (5.11) so that

$$\tilde{\epsilon} = \frac{\sin^2(\sqrt{\epsilon} k_0 h/2)}{\sin^2(k_0 h/2)} \quad (9.62)$$

is the effective relative permittivity on the numerical grid.

9.4.4 Computational boundaries

Reflecting and periodic boundaries for the NS-FD algorithm are given by Eqs. (9.15) and (9.16). Following Section 6.1.4, the NS-ABC for the NS-Yee algorithm is

$$B'_y|_{N+1/2}^{\tau+1/2} = B'_y|_{N-1/2}^{\tau-1/2} + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) (B'_y|_{N+1/2}^{\tau} - B'_y|_{N-1/2}^{\tau+1}), \quad (9.63a)$$

$$E_z|_0^{\tau+1} = E_z|_1^{\tau} - \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) (E_z|_1^{\tau+1} - E_z|_0^{\tau}), \quad (9.63b)$$

where

$$\tilde{v}_1 = \frac{\tan(\omega \Delta t/2)}{\tan(k \Delta x/2)}, \quad (9.64)$$

and k is the wavenumber in the boundary region. If $\omega \Delta t/k \Delta x = 1$, then $\tilde{v}_1 = 1$ and Eq. (9.63) reduces to the perfect ABC of Eq. (9.34).

In Program MC9.3, we implement the S- and NS-Yee algorithms with a point source and with the S-Mur and NS-Mur ABCs, respectively. The calculations are compared with the analytic expressions for the electromagnetic fields derived in Appendix 9.1.

Important Topics of Chapter 9

- The Yee algorithm in one dimension
- The NS-Yee algorithm
- Computational boundaries
- Effective permittivity on the grid

Appendix 9.1 Analytic Solution of Maxwell's 1D Equations for a Point Source Current

When the electromagnetic fields are generated by a source current in a homogeneous nonconductive medium, Maxwell's Eqs. (9.25) (repeated below) become

$$\mu \partial_t H_y = \partial_x E_z, \quad (A9.1.1a)$$

$$\varepsilon \partial_t E_z = \partial_x H_y - J_{s,z}. \quad (A9.1.1b)$$

They yield the inhomogeneous wave equations:

$$\left(\partial_t^2 - \frac{1}{\varepsilon \mu} \partial_x^2 \right) H_y = -\frac{1}{\varepsilon \mu} \partial_x J_{s,z}, \quad (A9.1.2a)$$

$$\left(\partial_t^2 - \frac{1}{\varepsilon \mu} \partial_x^2 \right) E_z = -\frac{1}{\varepsilon} \partial_t J_{s,z} - \frac{1}{\varepsilon} \partial_t J_{s,z}. \quad (A9.1.2b)$$

For simplicity, let us take $\varepsilon = 1$ in the medium in which the source current is immersed, so that $\mu = 1/\nu^2$. Then, Eq. (A9.2.1) becomes

$$(\partial_t^2 - \nu^2 \partial_x^2) H_y = -\nu^2 \partial_x J_{s,z}, \quad (A9.1.3a)$$

$$(\partial_t^2 - \nu^2 \partial_x^2) E_z = -\partial_t J_{s,z}. \quad (A9.1.3b)$$

Take $J_{s,z}(x, t) = \delta(x)j(t)$, where $j(t) = 0$ for $t \leq 0$. Wave Eq. (A9.1.3) can be solved using the Green's function derived in Appendix 4.4, given by

$$G(x - x', t - t') = \frac{1}{2v} \Theta[v(t - t') - |x - x'|]. \quad (\text{A9.1.4})$$

Magnetic field

The Green's function solution for H_y is given by

$$\begin{aligned} H_y(x, t) &= -v^2 \frac{1}{2v} \int_{-\infty}^{\infty} dt' j(t') \int_{-\infty}^{\infty} dx' \Theta[v(t - t') - |x - x'|] \frac{d}{dx'} \delta(x') \\ &= -\frac{v}{2} \int_{-\infty}^{\infty} dt' j(t') \int_{-\infty}^{\infty} dx' \Theta[(t - t') - |x - x'|/v] \frac{d}{dx'} \delta(x'), \end{aligned} \quad (\text{A9.1.5})$$

where we have used the equivalence $\Theta[v(t - t') - |x - x'|] = \Theta[(t - t') - |x - x'|/v]$.

Note 9.1

Although $\Theta(vt - |x|) = \Theta(t - |x|/v)$ for numerical evaluation, $\Theta(vt - |x|) \neq \Theta(t - |x|/v)$ when these expressions are differentiated. See Eqs. (4.68) and (A4.4.17).

Next, using Eq. (A3.4.6), here re-expressed in the form

$$\int_{-\infty}^{\infty} dx f(x) \frac{d}{dx} \delta(x) = -\frac{d}{dx} f(x)|_{x=0}, \quad (\text{A9.1.6})$$

we obtain

$$H_y(x, t) = \frac{v}{2} \int_{-\infty}^{\infty} dt' j(t') \frac{\partial}{\partial x'} \Theta[(t - t') - |x - x'|/v]|_{x'=0}. \quad (\text{A9.1.7})$$

Using Eq. (A3.4.28), together with $\partial_x \Theta(x) = \delta(x)$, and the fact that $\partial_x |x| = \text{sgn}(x)$ for $x \neq 0$, we find that

$$\frac{\partial}{\partial x'} \Theta[(t - t') - |x - x'|/v] = \delta[(t - t') - |x - x'|/v] \frac{1}{v} \text{sgn}(x - x'), \quad (\text{A9.1.8})$$

and hence

$$\begin{aligned} H_y(x, t) &= \frac{1}{2} \text{sgn}(x) \int_{-\infty}^{\infty} dt' j(t') \delta[(t - t') - |x|/v] \\ &= \frac{1}{2} \text{sgn}(x) j(t - |x|/v), \end{aligned} \quad (\text{A9.1.9})$$

where it must be kept in mind that $j(t) = 0$ for $t \leq 0$.

Electric field

E_z is given by

$$\begin{aligned}
 E_z(x, t) &= -\frac{1}{2v} \int_{-\infty}^{\infty} dt' \frac{d}{dt'} j(t') \int_{-\infty}^{\infty} dx' \Theta[v(t-t') - |x-x'|] \delta(x') \\
 &= -\frac{1}{2v} \int_{-\infty}^{\infty} dt' \frac{d}{dt'} j(t') \Theta[(t-t') - |x|/v] \\
 &= -\frac{1}{2v} j(t - |x|/v),
 \end{aligned} \tag{A9.1.10}$$

using the fact that $j(t) = 0$ for $t \leq 0$.

Evaluating the ratio H_y/E_z , we find that

$$\begin{aligned}
 \frac{H_y(x, t)}{E_z(x, t)} &= -v \operatorname{sgn}(x) \\
 &= -\operatorname{sgn}(x) \sqrt{\frac{\epsilon}{\mu}}.
 \end{aligned} \tag{A9.1.11}$$

Example calculation

Let

$$j(t) = \Theta(t) e^{i\omega t}; \tag{A9.1.12}$$

then,

$$H_y(x, t) = \frac{1}{2} \operatorname{sgn}(x) \Theta(t - |x|/v) e^{i(\omega t - k|x|)}, \tag{A9.1.13}$$

where $k = \omega/v$, and

$$\begin{aligned}
 E_z(x, t) &= -\frac{1}{2v} j(t - |x|/v) \\
 &= -\frac{1}{2v} \Theta(t - |x|/v) e^{i(\omega t - k|x|)},
 \end{aligned} \tag{A9.1.14}$$

where the step function is inserted to ensure that $E_z(x, t) = 0$ and $H_y(x, t) = 0$ for both $t \leq 0$ and $t < |x|/v$.

Appendix 9.2 Computer Program in Pseudocode

Implementation of the standard Yee algorithm [Eq. (9.13)] is as follows:

$$H_y|_{\chi+1/2}^{\tau+1/2} = H_y|_{\chi+1/2}^{\tau-1/2} + \frac{\Delta t}{\mu \Delta x} \left(E_z|_{\chi+1}^{\tau} - E_z|_{\chi}^{\tau} \right) \text{ for } 0 \leq \chi \leq N-1, \tag{A9.2.1}$$

$$E_z|_{\chi}^{\tau+1} = E_z|_{\chi}^{\tau} + \frac{\Delta t}{\varepsilon \Delta x} \left(H_y|_{\chi+1/2}^{\tau+1/2} - H_y|_{\chi-1/2}^{\tau+1/2} \right) \quad \text{for } 1 \leq \chi \leq N. \quad (\text{A9.2.2})$$

H_y and E_z are laid out on the grid as shown in Fig. 9.1.

Program initialization

The first step is to initialize the fields. We take the initial field to be a pulse given by

$$\varphi_0(x, t) = p(x \mp vt) \psi(x \mp vt), \quad (\text{A9.2.3})$$

where

$$\begin{aligned} p(x) &= 1 & \text{for } x_1 < x < x_2, \\ &= 0 & \text{otherwise,} \end{aligned} \quad (\text{A9.2.4})$$

and ψ is a waveform.

E_z is defined on $0 \leq x \leq N\Delta x$ and H_y on $\Delta x/2 \leq x \leq (N + 1/2)\Delta x$, so we take

$$E_z|_{\chi}^0 = \varphi_0(\chi \Delta x, 0), \quad (\text{A9.2.5a})$$

$$H_y|_{\chi+1/2}^{-1/2} = \mp \sqrt{\frac{\varepsilon}{\mu}} \varphi_0[(\chi + 1/2)\Delta x, -1/2]. \quad (\text{A9.2.5b})$$

It is often the case that μ very nearly equals its free-space value (except in different non-ferromagnetic media). Following the discussion in Section 8.2, we take the value of μ to be $\mu_0 = 1/\nu_0^2$ everywhere, where ν_0 is the propagation velocity in FDTD. If the medium is vacuum, then we can set $\nu_0 = 1$. In the simple program that follows, we also take $\varepsilon = \varepsilon_0 = 1$ so that we compute propagation in free space.

In the program, both $H_y \rightarrow \mathbf{H}$ and $E_z \rightarrow \mathbf{E}$ are column matrices with integer indices running from $0, 1, \dots, N$. Following the coding conventions of the previous chapters, we take $\Delta x = \Delta t = 1$. The initialization of program PC9.1 is given below in pseudocode.

Program PC9.1: Yee Algorithm in One Dimension

Initialization

for $ix = 0, 1, \dots, N$

$$E_{ix} = \varphi_0(ix, 0)$$

$$H_{ix} = \mp \sqrt{\frac{\varepsilon}{\mu}} \varphi_0(ix + 0.5, -0.5).$$

Yee Algorithm with the S-Mur Absorbing Computational Boundary

$$\begin{array}{l}
 \text{FDTD\_A}(\Psi) := \begin{array}{l}
 \begin{array}{l}
 \text{input} \\
 \Psi = \begin{pmatrix} H \\ E \\ t \end{pmatrix} = \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{pmatrix}
 \end{array} \\
 \begin{array}{l}
 H \leftarrow \Psi_0 \quad \leftarrow \text{input fields} \\
 E \leftarrow \Psi_1 \\
 t \leftarrow \Psi_2 \quad \leftarrow \text{time}
 \end{array} \\
 bE \leftarrow -E_1 + w \cdot E_0 \quad \leftarrow \text{use to compute E on the left boundary of the CD} \\
 bH \leftarrow -H_{N-1} + w \cdot H_N \quad \leftarrow \text{use to compute H on the right boundary of the CD} \\
 \text{for } i \in 0..N-1 \\
 \quad H_i \leftarrow H_i + \frac{1}{\mu_0} \cdot (E_{i+1} - E_i) \quad \leftarrow \text{update H in the interior of the CD} \\
 \quad H_N \leftarrow bH - w \cdot H_{N-1} \quad \leftarrow \text{update H on the right boundary of the CD} \\
 \text{for } i \in 1..N \\
 \quad E_i \leftarrow E_i + \frac{1}{\epsilon_0} \cdot (H_i - H_{i-1}) \quad \leftarrow \text{update E in the interior of the CD} \\
 \quad E_0 \leftarrow bE - w \cdot E_1 \quad \leftarrow \text{update E on the left boundary of the CD} \\
 \begin{pmatrix} H \\ E \\ t+1 \end{pmatrix} \quad \leftarrow \text{output: updated E and H field and updated time}
 \end{array}
 \end{array}$$

The output of the FDTD program can be inserted into a time loop to compute as many steps as desired. In our programs we periodically write to file for visualization. See Program MC9.1 for an example.

Yee Algorithm with Reflecting Computational Boundary

$$\begin{array}{l}
 \text{FDTD\_R}(\Psi) := \begin{array}{l}
 H \leftarrow \Psi_0 \\
 E \leftarrow \Psi_1 \\
 t \leftarrow \Psi_2 \\
 \text{for } i \in 0..N-1 \\
 \quad H_i \leftarrow H_i + \frac{1}{\mu_0} \cdot (E_{i+1} - E_i) \\
 \quad H_N \leftarrow 0 \\
 \text{for } i \in 1..N \\
 \quad E_i \leftarrow E_i + \frac{1}{\epsilon_0} \cdot (H_i - H_{i-1}) \\
 \quad E_0 \leftarrow 0 \\
 \begin{pmatrix} H \\ E \\ t+1 \end{pmatrix}
 \end{array}
 \end{array}$$

Yee Algorithm with Periodic Computational Boundary

$$\begin{array}{l}
 \text{FDTD\_P}(\Psi) := \begin{array}{l}
 H \leftarrow \Psi_0 \\
 E \leftarrow \Psi_1 \\
 t \leftarrow \Psi_2 \\
 \text{for } i \in 0..N-1 \\
 \quad H_i \leftarrow H_i + \frac{1}{\mu_0} \cdot (E_{i+1} - E_i) \\
 \quad H_N \leftarrow H_0 \\
 \text{for } i \in 1..N \\
 \quad E_i \leftarrow E_i + \frac{1}{\epsilon_0} \cdot (H_i - H_{i-1}) \\
 \quad E_0 \leftarrow E_N \\
 \begin{pmatrix} H \\ E \\ t+1 \end{pmatrix}
 \end{array}
 \end{array}$$

The output of these programs can also be inserted into a time loop to compute as many steps as desired.

See Program MC9.1 for a working Mathcad program.

References

1. K. S. Yee, "Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media," *IEEE Transactions on Antennas and Propagation* **14**(3), 302–307 (1966).

Chapter 10

The Yee Algorithm in Two and Three Dimensions

In this chapter we extend the 1D Yee algorithm developed in the previous chapter to two and three dimensions. Higher dimensions give rise to a few additional complications, especially on the computational boundary, but otherwise the development is straightforward.

10.1 General Development

In a linear nonconducting medium, including a source current, Maxwell's equations are

$$\mu \partial_t \mathbf{H} = -\nabla \times \mathbf{E}, \quad (10.1a)$$

$$\varepsilon \partial_t \mathbf{E} = \nabla \times \mathbf{H} - \mathbf{J}_s. \quad (10.1b)$$

Taking $\Delta x = \Delta y = \Delta z = h$ and defining the vector difference operator $\mathbf{d} = (d_x, d_y, d_z)$, we have the approximation

$$\nabla \cong \frac{\mathbf{d}}{h}. \quad (10.2)$$

Following the development in one dimension (see Section 9.2), the basic standard Yee model is

$$\mu(\mathbf{x}_H) \, d_t \mathbf{H}(\mathbf{x}_H, t) = -\frac{\Delta t}{h} \mathbf{d} \times \mathbf{E}(\mathbf{x}_H, t), \quad (10.3a)$$

$$\varepsilon(\mathbf{x}_E) \, d_t \mathbf{E}(\mathbf{x}_E, t + \Delta t/2) = \frac{\Delta t}{h} \mathbf{d} \times \mathbf{H}(\mathbf{x}_E, t + \Delta t/2) - \mathbf{J}_s(\mathbf{x}_E, t + \Delta t/2), \quad (10.3b)$$

where $\mathbf{x} = (x, y, z)$. The components of $\mathbf{H}$ are specified at positions $\mathbf{x}_H$, and those of $\mathbf{E}$ and $\mathbf{J}_s$ at $\mathbf{x}_E$. As in one dimension, these positions are chosen so that the derivatives can be modeled by central finite differences. There is more

than one possible set of choices for $\mathbf{x}_H$ and $\mathbf{x}_E$. In addition, ε and μ are specified at different positions for each component of $\mathbf{H}$ and $\mathbf{E}$. On a fine grid it might be a good approximation to ignore this, but on a coarse grid, especially near a resonance, appreciable error can arise. Expanding $d_t\mathbf{H}$ and $d_t\mathbf{E}$, and solving for $\mathbf{H}(\mathbf{x}_H, t + \Delta t/2)$ and $\mathbf{E}(\mathbf{x}_E, t + \Delta t)$, the standard Yee algorithm becomes

$$\mathbf{H}(\mathbf{x}_H, t + \Delta t/2) = \mathbf{H}(\mathbf{x}_H, t - \Delta t/2) - \frac{1}{\mu(\mathbf{x}_H)} \frac{\Delta t}{h} \mathbf{d} \times \mathbf{E}(\mathbf{x}_H, t), \quad (10.4a)$$

$$\begin{aligned} \mathbf{E}(\mathbf{x}_E, t + \Delta t) &= \mathbf{E}(\mathbf{x}_E, t) + \frac{1}{\varepsilon(\mathbf{x}_E)} \\ &\times \left[\frac{\Delta t}{h} \mathbf{d} \times \mathbf{H}(\mathbf{x}_E, t + \Delta t/2) - \Delta t \mathbf{J}_s(\mathbf{x}_E, t + \Delta t/2) \right]. \end{aligned} \quad (10.4b)$$

Following Chapter 9, when conductivity is included, Eq. (10.4b) becomes

$$\begin{aligned} \mathbf{E}(\mathbf{x}_E, t + \Delta t) &= \left[\frac{C^-(\mathbf{x}_E)}{C^+(\mathbf{x}_E)} \right] \mathbf{E}(\mathbf{x}_E, t) + \frac{1}{C^+(\mathbf{x}_E)} \frac{1}{\varepsilon(\mathbf{x}_E)} \\ &\times \left[\frac{\Delta t}{h} \mathbf{d} \times \mathbf{H}(\mathbf{x}_E, t + \Delta t/2) - \Delta t \mathbf{J}_s(\mathbf{x}_E, t + \Delta t/2) \right], \end{aligned} \quad (10.4c)$$

where $C^\pm(\mathbf{x}_E) = 1 \pm \sigma(\mathbf{x}_E)\Delta t/2\varepsilon(\mathbf{x}_E)$.

Nonstandard Yee algorithms

A complication arises when we try to extend the nonstandard methodology of Chapter 9 to more than one dimension. While $\mathbf{d} \bullet \mathbf{d} = \mathbf{d}^2$, there is no NS difference operator $\mathbf{d}'$ such that $\mathbf{d}' \bullet \mathbf{d}' = \tilde{\mathbf{d}}^2$. We can however define $\tilde{\mathbf{d}}$ (see Sections 1.4 and 1.5) such that $\mathbf{d} \bullet \tilde{\mathbf{d}} = \tilde{\mathbf{d}} \bullet \mathbf{d} = \tilde{\mathbf{d}}^2$ (but $\tilde{\mathbf{d}} \bullet \tilde{\mathbf{d}} \neq \tilde{\mathbf{d}}^2$). We find that

$$\tilde{\mathbf{d}} = \mathbf{d} + \left[\frac{1}{12} + \frac{(kh)^2}{360} \right] \begin{bmatrix} d_x(d_y^2 + d_z^2) \\ d_y(d_x^2 + d_z^2) \\ d_z(d_x^2 + d_y^2) \end{bmatrix} + \frac{1}{90} \begin{bmatrix} d_x(d_y^2 d_z^2) \\ d_y(d_x^2 d_z^2) \\ d_z(d_x^2 d_y^2) \end{bmatrix}, \quad (10.5)$$

where the column matrices represent vector difference operators. The 2D form of $\tilde{\mathbf{d}}$ is obtained by setting $d_z = 0$ in Eq. (10.5).

Following Chapter 9, we define $\mathbf{B}' = \mu\mathbf{H}h/\Delta t$, and the NS-Yee model with a source current becomes

$$d_t\mathbf{B}'(\mathbf{x}_H, t) = -\mathbf{d} \times \mathbf{E}(\mathbf{x}_H, t), \quad (10.6a)$$

$$d_t\mathbf{E}(\mathbf{x}_E, t + \Delta t/2) = \tilde{\mathbf{d}}^2 \times \mathbf{B}'(\mathbf{x}_E, t + \Delta t/2) - \tilde{\mathbf{J}}_s(\mathbf{x}_E, t + \Delta t/2), \quad (10.6b)$$

from which we obtain the NS-Yee algorithm,

$$\mathbf{B}'(\mathbf{x}_H, t + \Delta t/2) = \mathbf{B}'(\mathbf{x}_H, t - \Delta t/2) - \mathbf{d} \times \mathbf{E}(\mathbf{x}_H, t), \quad (10.7a)$$

$$\begin{aligned} \mathbf{E}(\mathbf{x}_E, t + \Delta t) &= \mathbf{E}(\mathbf{x}_E, t) + \tilde{v}^2 \mathbf{d} \times \mathbf{H}'(\mathbf{x}_E, t + \Delta t/2) \\ &\quad - \tilde{\mathbf{J}}_s(\mathbf{x}_E, t + \Delta t/2), \end{aligned} \quad (10.7b)$$

where $\tilde{\mathbf{J}}_s$ is the nonstandard model of the source current.

Taking $\tilde{\mathbf{J}}_s = 0$ in a conducting dielectric (following Chapter 9), Eq. (10.7a) remains unchanged, while Eq. (10.7b) becomes

$$\mathbf{E}(\mathbf{x}_E, t + \Delta t) = \frac{1}{\tilde{C}^+(\mathbf{x}_E)} [\tilde{C}^-(\mathbf{x}_E) \mathbf{E}(\mathbf{x}_E, t) + \tilde{v}'^2(\mathbf{x}_E) \mathbf{d} \times \mathbf{B}'(\mathbf{x}_E, t + \Delta t/2)], \quad (10.8)$$

where

$$\tilde{\alpha}' = -\tan(\omega \Delta t/2) \frac{\sin(k'_r h) \sinh(k'_i h)}{1 - \cos(k'_r h) \cosh(k'_i h)}, \quad (10.9a)$$

$\tilde{C}^\pm(\mathbf{x}_E) = 1 \pm \tilde{\alpha}'(\mathbf{x}_E)$, and

$$\tilde{v}'^2 = \frac{2 \sin^2(\omega \Delta t/2)}{1 - \cos(k'_r h) \cosh(k'_i h)}; \quad (10.9b)$$

$k' = k'_r + i k'_i$ is given by

$$k' = \frac{k}{\sqrt{2\omega}} \left[\left(\sqrt{\omega^2 + \sigma^2/\varepsilon^2} + \omega \right)^{1/2} - i \left(\sqrt{\omega^2 + \sigma^2/\varepsilon^2} - \omega \right)^{1/2} \right]. \quad (10.10)$$

Assuming that the electromagnetic fields are generated in a nonconducting medium, we omit the case of a source current embedded in a conducting material.

10.2 Implementation in Two Dimensions

Often we want to compute propagation through or scattering off of structures that are invariant (or can be approximately modeled as such) along one of the Cartesian axes, for example, an infinitely long cylinder centered on the z axis. Taking ε and μ to be invariant in the z direction, the total electromagnetic field can be expressed as a superposition of two sets of orthogonally polarized plane waves, the TE (transverse electric) mode and the TM (transverse

magnetic) mode. Since different communities use different definitions, one should always define TE and TM. In this book we adopt the definitions used by most of the optics community.

10.2.1 TM mode

We define TM polarization by

$$H_x = H_y = E_z = 0; \quad (10.11)$$

thus, $H_z(x, y, t) \neq 0$, and $\mathbf{H}$ is polarized *transverse* to the x - y plane (hence parallel to the z axis), while $E_x(x, y, t) \neq 0$, and $E_y(x, y, t) \neq 0$ so that $\mathbf{E}$ is parallel to the x - y plane.

Maxwell's equations in a linear nonconducting dielectric medium then reduce to

$$\mu \partial_t H_z = -\partial_x E_y + \partial_y E_x, \quad (10.12a)$$

$$\varepsilon \partial_t E_x = \partial_y H_z - J_{s,x}, \quad (10.12b)$$

$$\varepsilon \partial_t E_y = -\partial_x H_z - J_{s,y}. \quad (10.12c)$$

Standard Yee algorithm

Let us discretize space-time by taking $t = \tau \Delta t$ ($\tau = 0, 1, 2, \dots$) and $\mathbf{x} = (x, y) = (\mathbf{x}, y)h = \mathbf{x}h$, ($\mathbf{x} = 0, 1, \dots, \mathbf{x}_b$ and $y = 0, 1, \dots, y_b$), where $\Delta x = \Delta y = h$. To implement the Yee model [Eq. (10.3)] in a usable form, we must first decide the positions of the electromagnetic field components on the grid. There are several possible choices for $\mathbf{x}_H$ and $\mathbf{x}_E$. Let us choose

$$\mathbf{x}_{Hz} = (\mathbf{x}, y)h, \quad (10.13a)$$

$$\mathbf{x}_{Ex} = (\mathbf{x}, y + 1/2)h, \quad (10.13b)$$

$$\mathbf{x}_{Ey} = (\mathbf{x} + 1/2, y)h, \quad (10.13c)$$

as shown in Fig. 10.1.

From the Yee model we derive the standard (S) Yee algorithm on $(\mathbf{x} = 0, \dots, \mathbf{x}_b) \times (y = 0, \dots, y_b)$:

$$H_z \Big|_{\mathbf{x}, y}^{\tau+1/2} = H_z \Big|_{\mathbf{x}, y}^{\tau-1/2} + \frac{1}{\mu_{\mathbf{x}, y}} \frac{\Delta t}{h} \left(-d_x E_y \Big|_{\mathbf{x}, y}^{\tau} + d_y E_x \Big|_{\mathbf{x}, y}^{\tau} \right), \quad (10.14a)$$

$$E_x \Big|_{\mathbf{x}, y+1/2}^{\tau+1} = E_x \Big|_{\mathbf{x}, y+1/2}^{\tau} + \frac{1}{\varepsilon_{\mathbf{x}, y+1/2}} \left(\frac{\Delta t}{h} d_y H_z \Big|_{\mathbf{x}, y+1/2}^{\tau+1/2} - \Delta t J_{s,x} \Big|_{\mathbf{x}, y+1/2}^{\tau+1/2} \right), \quad (10.14b)$$

$$E_y \Big|_{\mathbf{x}+1/2, y}^{\tau+1} = E_y \Big|_{\mathbf{x}+1/2, y}^{\tau} - \frac{1}{\varepsilon_{\mathbf{x}+1/2, y}} \left(\frac{\Delta t}{h} d_x H_z \Big|_{\mathbf{x}+1/2, y}^{\tau+1/2} - \Delta t J_{s,y} \Big|_{\mathbf{x}+1/2, y}^{\tau+1/2} \right). \quad (10.14c)$$

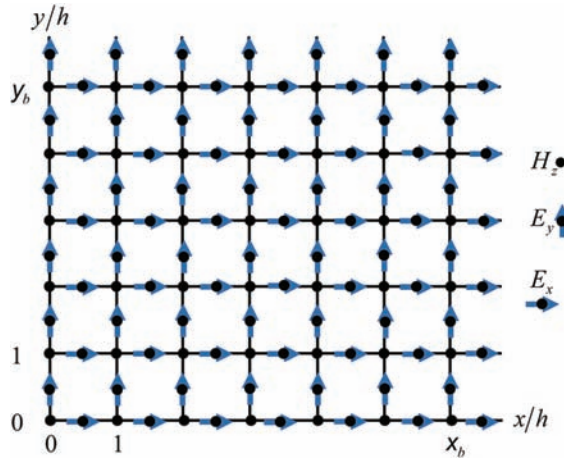


Figure 10.1 Layout of the electromagnetic fields in the TM mode.

As it stands, algorithm Eq. (10.14) does not tell us how to compute the fields on the computational boundary. For this we need to add auxiliary conditions.

Periodic computational boundary

Defining

$$E_y|_{-1/2,y}^{\tau} \equiv E_y|_{x_b+1/2,y}^{\tau} \quad \text{and} \quad E_x|_{x,-1/2}^{\tau} \equiv E_x|_{x,y_b+1/2}^{\tau}, \quad (10.15a)$$

we obtain $d_x E_y|_{0,y}^{\tau} = E_y|_{1/2,y}^{\tau} - E_y|_{x_b+1/2,y}^{\tau}$ and $d_y E_x|_{x,0}^{\tau} = E_x|_{x,1/2}^{\tau} - E_x|_{x,y_b+1/2}^{\tau}$ in Eq. (10.14a). Similarly,

$$H_z|_{x,y_b+1}^{\tau+1/2} \equiv H_z|_{x,0}^{\tau+1/2} \quad (10.15b)$$

gives $d_y H_z|_{x,y_b+1/2}^{\tau+1/2} = H_z|_{x,0}^{\tau+1/2} - H_z|_{x,y_b}^{\tau+1/2}$ in Eq. (10.14b), and

$$H_z|_{x_b+1,y}^{\tau+1/2} \equiv H_z|_{0,y}^{\tau+1/2} \Rightarrow \quad (10.15c)$$

gives $d_x H_z|_{x_b+1/2,y}^{\tau+1/2} = H_z|_{0,y}^{\tau+1/2} - H_z|_{x_b,y}^{\tau+1/2}$ in Eq. (10.14c).

Reflecting computational boundary

$$E_y \Big|_{-1/2, y}^{\tau} \equiv 0 \quad \text{and} \quad E_x \Big|_{x, -1/2}^{\tau} \equiv 0, \quad (10.16a)$$

$$H_z \Big|_{x, y_b+1}^{\tau+1/2} \equiv 0, \quad (10.16b)$$

$$H_z \Big|_{x_b+1, y}^{\tau+1/2} \equiv 0 \quad (10.16c)$$

in Eqs. (10.14a), (b), and (c), respectively.

Standard Mur absorbing boundary condition

There are several different ways to implement the Mur absorbing boundary condition (ABC). Since H_z is computed first in Eq. (10.14), we choose to enforce it on H_z only.

For example, on the left computational boundary (see Fig. 10.1), we enforce the ABC at $x = 1$; thus, in Eq. (7.93a) we set $b = 1$ and $i = 2$:

$$\begin{aligned} \psi_{1,y}^{\tau+1} = & \psi_{1,y}^{\tau} + \left(\psi_{2,y}^{\tau} - \psi_{2,y}^{\tau-1} \right) + \left(\frac{1-u}{1+u} \right) \left[\left(\psi_{1,y}^{\tau} - \psi_{1,y}^{\tau-1} \right) - \left(\psi_{2,y}^{\tau+1} - \psi_{2,y}^{\tau} \right) \right] \\ & + \frac{1}{2} \left(\frac{u^2}{1+u} \right) d_y^2 \left(\psi_{1,y}^{\tau} + \psi_{2,y}^{\tau} \right), \end{aligned} \quad (10.17)$$

where $u = \nu \Delta t / h$. Recasting this as a two-step process, we obtain

$$\begin{aligned} d_{\tau} \psi_{1,y}^{\tau+1/2} = & d_{\tau} \psi_{2,y}^{\tau-1/2} + \left(\frac{1-u}{1+u} \right) (d_{\tau} \psi_{1,y}^{\tau-1/2} - d_{\tau} \psi_{2,y}^{\tau+1/2}) \\ & + \frac{1}{2} \left(\frac{u^2}{1+u} \right) d_y^2 (\psi_{1,y}^{\tau} + \psi_{2,y}^{\tau}), \end{aligned} \quad (10.18a)$$

$$\psi_{1,y}^{\tau+1} = \psi_{1,y}^{\tau} + d_{\tau} \psi_{1,y}^{\tau+1/2}. \quad (10.18b)$$

Now putting $\psi_{x,y}^{\tau} \rightarrow H_z \Big|_{x,y}^{\tau+1/2}$, Eq. (10.18a) becomes

$$\begin{aligned} d_{\tau} H_z \Big|_{1,y}^{\tau} = & d_{\tau} H_z \Big|_{2,y}^{\tau-1} + \left(\frac{1-u}{1+u} \right) \left(d_{\tau} H_z \Big|_{1,y}^{\tau-1} - d_{\tau} H_z \Big|_{2,y}^{\tau} \right) \\ & + \frac{1}{2} \left(\frac{u^2}{1+u} \right) d_y^2 \left(H_z \Big|_{1,y}^{\tau-1/2} + H_z \Big|_{2,y}^{\tau-1/2} \right). \end{aligned} \quad (10.19a)$$

After this update, we set $H_z \Big|_{0,y}^{\tau+1/2} = 0$, and finally, the H_z field is updated using

$$H_z|_{x,y}^{\tau+1/2} = H_z|_{x,y}^{\tau-1/2} + d_\tau H_z|_{x,y}^\tau \quad (10.19b)$$

at all points.

Similarly, taking $b = 1$ and $i = 2$, and putting $\psi_{x,y}^\tau \rightarrow H_z|_{x,y}^{\tau+1/2}$ in Eq. (7.93b), we obtain an ABC on the bottom boundary:

$$\begin{aligned} d_\tau H_z|_{x,1}^\tau &= d_\tau H_z|_{x,1}^{\tau-1} + \left(\frac{1-u}{1+u}\right) \left(d_\tau H_z|_{x,1}^{\tau-1} - d_\tau H_z|_{x,2}^\tau\right) \\ &\quad + \frac{1}{2} \left(\frac{u^2}{1+u}\right) d_x^2 \left(H_z|_{x,1}^{\tau-1/2} + H_z|_{x,2}^{\tau-1/2}\right). \end{aligned} \quad (10.19c)$$

After this update, we set $H_z|_{x,0}^{\tau+1/2} = 0$, and the final H_z field is updated at all points using

$$H_z|_{x,y}^{\tau+1/2} = H_z|_{x,y}^{\tau-1/2} + d_\tau H_z|_{x,y}^\tau. \quad (10.19d)$$

There is no need to formulate an ABC for the electric field because it is computed from H_z .

Note 10.1

If not implemented correctly, the Mur ABC can be numerically unstable. Program MC10.1 implements the basic Yee algorithm with the Mur ABC. We have verified its long-term stability. The stability analysis of Appendix 7.2 applies only to an infinite boundary. Thus, long-run computational verifications are essential.

The advantage of the Mur ABC, especially its nonstandard version, is its simplicity and low computational cost. In the version given in Program MC10.1, only three layers are needed to give reasonable absorption. When this is not sufficient, the perfectly matched layer (PML) methodology is available. The PML method is more complicated and costly to implement than the Mur ABC, but it is currently the best available. The theory and implementation are developed in Refs. 1–3. The methodologies of Refs. 4–7 are another option.

S-FDTD with conductivity

Taking $J_{s,x} = J_{s,y} = 0$, conductivity can be straightforwardly incorporated following the 1D developments of Section 9.4.2. Equation (10.14a) remains unchanged, while Eqs. (10.14b) and (c) become

$$E_x|_{x,y+1/2}^{\tau+1} = \frac{1}{C_{x,y+1/2}^+} \left(C_{x,y+1/2}^- E_x|_{x,y+1/2}^\tau + \frac{1}{\varepsilon_{x,y+1/2}} \frac{\Delta t}{h} d_y H_z|_{x,y+1/2}^{\tau+1/2} \right), \quad (10.20a)$$

$$E_y|_{x+1/2,y}^{\tau+1} = \frac{1}{C_{x+1/2,y}^+} \left(C_{x+1/2,y}^- E_y|_{x+1/2,y}^\tau - \frac{1}{\varepsilon_{x+1/2,y}} \frac{\Delta t}{h} d_x H_z|_{x+1/2,y}^{\tau+1/2} \right), \quad (10.20b)$$

where $C_{x,y}^\pm = 1 \pm \sigma_{x,y} \Delta t / 2\varepsilon_{x,y}$. We omit the case of a source current embedded in a conducting dielectric.

Nonstandard Yee algorithm

The NS-Yee algorithm is easily derived from the S-Yee algorithm:

$$B_z'|_{x,y}^{\tau+1/2} = B_z'|_{x,y}^{\tau-1/2} - d_x E_y|_{x,y}^\tau + d_y E_x|_{x,y}^\tau, \quad (10.21a)$$

$$E_x|_{x,y+1/2}^{\tau+1} = E_x|_{x,y+1/2}^\tau + \tilde{v}_{x,y+1/2}^2 \tilde{d}_y B_z'|_{x,y+1/2}^{\tau+1/2} - \tilde{J}_{s,x}|_{x,y+1/2}^{\tau+1/2}, \quad (10.21b)$$

$$E_y|_{x+1/2,y}^{\tau+1} = E_y|_{x+1/2,y}^\tau - \tilde{v}_{x+1/2,y}^2 \tilde{d}_x B_z'|_{x+1/2,y}^{\tau+1/2} - \tilde{J}_{s,y}|_{x+1/2,y}^{\tau+1/2}. \quad (10.21c)$$

For $\tilde{\mathbf{J}}_s = 0$, from Eq. (10.8), the NS-Yee algorithm for a conducting dielectric becomes

$$B_z'|_{x,y}^{\tau+1/2} = B_z'|_{x,y}^{\tau-1/2} - d_x E_y|_{x,y}^\tau + d_y E_x|_{x,y}^\tau, \quad (10.22a)$$

$$E_x|_{x,y+1/2}^{\tau+1} = \frac{1}{\tilde{C}_{x,y+1/2}^+} \left(\tilde{C}_{x,y+1/2}^- E_x|_{x,y+1/2}^\tau + \tilde{v}_{x,y+1/2}'^2 \tilde{d}_y B_z'|_{x,y+1/2}^{\tau+1/2} \right), \quad (10.22b)$$

$$E_y|_{x+1/2,y}^{\tau+1} = \frac{1}{\tilde{C}_{x+1/2,y}^+} \left(\tilde{C}_{x+1/2,y}^- E_y|_{x+1/2,y}^\tau - \tilde{v}_{x+1/2,y}'^2 \tilde{d}_x B_z'|_{x+1/2,y}^{\tau+1/2} \right). \quad (10.22c)$$

The ranges of (x, y) for each component are the same as those of Eq. (10.14). Periodic and reflecting computational boundaries are given by Eqs. (10.15) and (10.16). The NS absorbing boundary condition is obtained from Eq. (10.19) with the substitutions $u \rightarrow \tilde{v}_1$ and $u^2 \rightarrow \tilde{v}_2^2$, where $\tilde{v}_1$ and $\tilde{v}_2^2$ are given by Eq. (7.106). Its stability conditions are given in Appendix 7.2.

10.2.2 TE mode

The TE polarization is defined by

$$H_z = E_x = E_y = 0; \quad (10.23)$$

thus, $\mathbf{E}$ is polarized *transverse* to the x - y plane (hence, parallel to the z axis), and $\mathbf{H}$ is parallel to the x - y plane. Therefore, $H_x(x, y, t) \neq 0$, $H_y(x, y, t) \neq 0$, and $E_z(x, y, t) \neq 0$.

Maxwell's equations in a linear nonconducting dielectric medium then reduce to

$$\mu \partial_t H_x = -\partial_y E_z, \quad (10.24a)$$

$$\mu \partial_t H_y = \partial_x E_z, \quad (10.24b)$$

$$\varepsilon \partial_t E_z = \partial_x H_y - \partial_y H_x. \quad (10.24c)$$

Standard Yee algorithm

We now develop the Yee algorithm for the TE mode. Here we assume $\varepsilon(x, y)$ and $\mu(x, y)$ to be invariant along the z axis. Taking the positions of the electromagnetic field components to be (see Fig. 10.2)

$$\mathbf{x}_{E_z} = (x, y) h, \quad (10.25a)$$

$$\mathbf{x}_{H_x} = (x, y + 1/2) h, \quad (10.25b)$$

$$\mathbf{x}_{H_y} = (x + 1/2, y) h, \quad (10.25c)$$

on $(x = 0, \dots, x_b) \times (y = 0, \dots, y_b)$, the S-Yee algorithm becomes

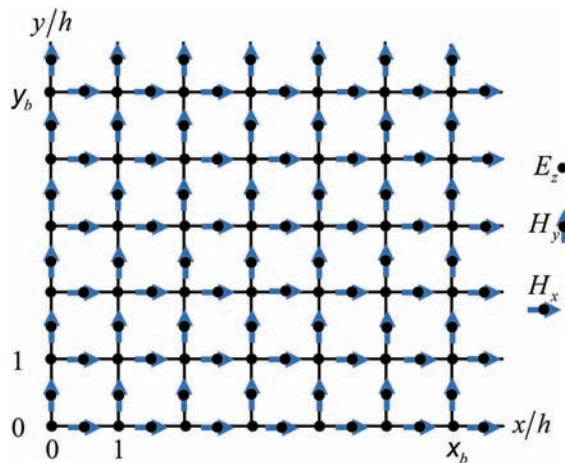


Figure 10.2 Layout of the electromagnetic fields in the TE mode.

$$H_x \Big|_{x,y+1/2}^{\tau+1/2} = H_x \Big|_{x,y+1/2}^{\tau-1/2} - \frac{1}{\mu_{x,y+1/2}} \frac{\Delta t}{h} d_y E_z \Big|_{x,y+1/2}^{\tau}, \quad (10.26a)$$

$$H_y \Big|_{x+1/2,y}^{\tau+1/2} = H_y \Big|_{x+1/2,y}^{\tau-1/2} + \frac{1}{\mu_{x+1/2,y}} \frac{\Delta t}{h} d_x E_z \Big|_{x+1/2,y}^{\tau}, \quad (10.26b)$$

$$E_z \Big|_{x,y}^{\tau+1} = E_z \Big|_{x,y}^{\tau} + \frac{1}{\varepsilon_{x,y}} \frac{\Delta t}{h} \left\{ d_x H_y \Big|_{x,y}^{\tau+1/2} - d_y H_x \Big|_{x,y}^{\tau+1/2} \right\}. \quad (10.26c)$$

The corresponding NS-Yee algorithm is given by

$$B'_x \Big|_{x,y+1/2}^{\tau+1/2} = B'_x \Big|_{x,y+1/2}^{\tau-1/2} - d_y E_z \Big|_{x,y+1/2}^{\tau}, \quad (10.27a)$$

$$B'_y \Big|_{x+1/2,y}^{\tau+1/2} = B'_y \Big|_{x+1/2,y}^{\tau-1/2} + d_x E_z \Big|_{x+1/2,y}^{\tau}, \quad (10.27b)$$

$$E_z \Big|_{x,y}^{\tau+1} = E_z \Big|_{x,y}^{\tau} + \tilde{\nu}_{x,y}^2 \left(\tilde{d}_x H_y \Big|_{x,y}^{\tau+1/2} - \tilde{d}_y H_x \Big|_{x,y}^{\tau+1/2} \right). \quad (10.27c)$$

Computational boundaries

The computational boundaries can be handled in the same way as in Section 10.2.1.

Equivalence of the wave equation in E_z to Maxwell's equations for uniform μ

In many physical media, μ very nearly equals its vacuum value, while ε is different in different media.

Let B be a boundary between dielectric medium 1 and dielectric medium 2, where ε may be complex. Let $\hat{\tau}$ be a unit vector tangent to B at point $\mathbf{x}_B$ on B . Taking the electromagnetic fields in mediums 1 and 2 to be $(\mathbf{E}_1, \mathbf{H}_1)$ and $(\mathbf{E}_2, \mathbf{H}_2)$, respectively, the tangential components of $\mathbf{E}$ and $\mathbf{H}$ are continuous across B . For $\hat{\tau} = (\cos \theta, \sin \theta) = (\tau_x, \tau_y)$, the boundary conditions given by Eq. (8.46) reduce to $E_{1,z} = E_{2,z}$ and $\tau_x H_{1,x} + \tau_y H_{1,y} = \tau_x H_{2,x} + \tau_y H_{2,y}$. Without loss of generality, we can take $\hat{\tau}$ at $\mathbf{x}_B$ to be parallel to the x axis so that $\hat{\tau} = (1, 0)$ and the boundary conditions simplify to

$$E_{1,z} = E_{2,z}, \quad (10.28a)$$

$$H_{1,x} = H_{2,x}. \quad (10.28b)$$

If $H_{1,x} = H_{2,x}$, then $\partial_t H_{1,x} = \partial_t H_{2,x}$. If μ is constant across B , then from Eq. (10.24a), $\partial_y E_z$ is also constant across B so that

$$\partial_y E_{1,z} = \partial_y E_{2,z}. \quad (10.29)$$

Thus, the uniformity of μ implies that both E_z and its derivative normal to B are continuous. These are the same boundary conditions that the scalar

wave equation satisfies. Furthermore, multiplying Eq. (10.24c) by μ , taking the time derivative of both sides, and using Eq. (10.24a,b), we obtain the wave equation. Thus, E_z satisfies both the wave equation and its boundary conditions if μ is constant across B , even when ε is different on each side of the boundary.

Although the components of $\mathbf{H}$ satisfy the wave equation in each region of constant ε and μ on either side of B , they do not satisfy the wave equation across B and do not satisfy the boundary conditions of the wave equation on B . Hence, we cannot compute $\mathbf{H}$ using wave equation FDTD.

On the other hand, in the TM mode, if ε is constant everywhere, and $\mu = \mu(x, y)$ is invariant along the z axis, then Maxwell's equations for H_z together with its boundary conditions are equivalent to the wave equation for H_z together with its boundary conditions. In this case, the components of $\mathbf{E}$ do not satisfy the independent wave equations; however, this case does not often occur.

Numerical stability

The numerical stability constraints of the S- and NS-Yee algorithms are the same as those of the wave equation (see Chapter 7 and Appendices A7.1 and A7.2).

10.3 The Scattered Field

Assuming that $\mu = \mu_0$ everywhere, let a scatterer of permittivity ε_s relative to the ambient medium be illuminated by an incident electromagnetic field ($\mathbf{H}_0, \mathbf{E}_0$). By definition, the incident field obeys

$$\mu \partial_t \mathbf{H}_0 = -\nabla \times \mathbf{E}_0, \quad (10.30a)$$

$$\partial_t \mathbf{E}_0 = \nabla \times \mathbf{H}_0, \quad (10.30b)$$

where $\varepsilon = 1$ in the ambient medium. The total field is given by

$$\mu \partial_t \mathbf{H} = -\nabla \times \mathbf{E}, \quad (10.31a)$$

$$\varepsilon \partial_t \mathbf{E} = \nabla \times \mathbf{H}, \quad (10.31b)$$

where ε is the local value of electrical permittivity ($\varepsilon = \varepsilon_s$ inside the scatterer, $\varepsilon = 1$ outside). Subtracting Eq. (10.30) from Eq. (10.31) gives Maxwell's equations for the scattered field:

$$\mu \partial_t \mathbf{H}_s = -\nabla \times \mathbf{E}_s, \quad (10.32a)$$

$$\varepsilon \partial_t \mathbf{E}_s = -\nabla \times \mathbf{H}_s - (\varepsilon - 1) \partial_t \mathbf{E}_0, \quad (10.32b)$$

where

$$\mathbf{J}_s = (\varepsilon - 1)\partial_t \mathbf{E}_0 \quad (10.33)$$

is, effectively, a source current that arises due to the presence of the scatterer and vanishes outside of it.

Taking the incident electromagnetic field to be an infinite plane wave of unit amplitude, wavenumber $\mathbf{k}_0$, and angular frequency ω_0 , let

$$\mathbf{E}_0 = \hat{\mathbf{e}}_0 \psi_0, \quad (10.34)$$

where $\hat{\mathbf{e}}_0$ is a unit vector, and $\psi_0 = e^{i(\mathbf{k}_0 \cdot \mathbf{x} - \omega_0 t)}$. Because $\nabla \cdot \mathbf{E} = 0$ (charge density = 0),

$$\hat{\mathbf{e}}_0 \cdot \mathbf{k}_0 = 0; \quad (10.35)$$

then, from Eq. (10.33), the source of the scattered field is

$$\mathbf{J}_s = -i\omega_0(\varepsilon - 1)\hat{\mathbf{e}}_0 \psi_0. \quad (10.36)$$

Putting Eq. (10.34) into Eq. (10.30a) and taking the time dependence of $\mathbf{H}_0$ to be $e^{-i\omega_0 t}$, Maxwell's equation for the incident magnetic field becomes $\mu_0\omega_0\mathbf{H}_0 = k_0\hat{\mathbf{k}}_0 \times \hat{\mathbf{e}}_0 \psi_0$; hence, using the units introduced in Section 8.2.1,

$$\mathbf{H}_0 = \frac{\omega_0}{k_0} \hat{\mathbf{k}}_0 \times \hat{\mathbf{e}}_0 \psi_0 = c \hat{\mathbf{k}}_0 \times \mathbf{E}_0. \quad (10.37)$$

NS-FD model of the scattered field

The S-FD model and S-Yee algorithm follow obviously from previous developments, so we proceed to directly develop the NS-FD model.

Defining $\mathbf{B}'_0 = (h\mu/\Delta t)\mathbf{H}_0$, the NS-FD model for the incident field is

$$d_t \mathbf{B}'_0(\mathbf{x}, t) = -\mathbf{d} \times \mathbf{E}_0(\mathbf{x}, t), \quad (10.38a)$$

$$d_t \mathbf{E}_0(\mathbf{x}, t + \Delta t/2) = \tilde{v}_0^2 \tilde{\mathbf{d}} \times \mathbf{B}'_0(\mathbf{x}, t + \Delta t/2). \quad (10.38b)$$

Assuming uniform magnetic permeability, and following the 1D development in Section 9.3.3, the NSFD model of the total electromagnetic field is

$$d_t \mathbf{B}'(\mathbf{x}, t) = -\mathbf{d} \times \mathbf{E}(\mathbf{x}, t), \quad (10.39a)$$

$$d_t \mathbf{E}(\mathbf{x}, t + \Delta t/2) = \frac{\tilde{v}_0^2}{\tilde{\varepsilon}} \tilde{\mathbf{d}} \times \mathbf{B}'(\mathbf{x}, t + \Delta t/2), \quad (10.39b)$$

where the electrical permittivity on the grid in the NS model is given by

$$\tilde{\varepsilon} = \frac{\sin^2(\sqrt{\varepsilon} k_0 h/2)}{\sin^2(k_0 h/2)}. \quad (10.40)$$

Devil in the details

$\tilde{\mathbf{d}}$ in Eq. (10.38b) is evaluated in the ambient medium (which we call “free space”), while in Eq. (10.39b) it is evaluated using the local value of $\varepsilon = \varepsilon(\mathbf{x})$ [see Eq. (10.5)].

In Eq. (10.38b), let $\tilde{\mathbf{d}} = \tilde{\mathbf{d}}(1)$, and in Eq. (10.39b), let $\tilde{\mathbf{d}} = \tilde{\mathbf{d}}(\sqrt{\varepsilon})$. Defining

$$\Delta\tilde{\mathbf{d}} = \tilde{\mathbf{d}}(\sqrt{\varepsilon}) - \tilde{\mathbf{d}}(1), \quad (10.41)$$

and subtracting the NS-FDTD model of the incident field from that of the total field, we obtain

$$d_t \mathbf{B}'_s(\mathbf{x}, t) = -\mathbf{d} \times \mathbf{E}_s(\mathbf{x}, t), \quad (10.42a)$$

$$d_t \mathbf{E}_s(\mathbf{x}, t + \Delta t/2) = \frac{\tilde{v}_0^2}{\tilde{\varepsilon}} \tilde{\mathbf{d}}(\sqrt{\varepsilon}) \times \mathbf{B}'_s(\mathbf{x}, t + \Delta t/2) - \tilde{\mathbf{J}}_s(\mathbf{x}, t + \Delta t/2), \quad (10.42b)$$

where

$$\begin{aligned} \tilde{\mathbf{J}}_s(\mathbf{x}, t + \Delta t/2) = & \left(1 - \frac{1}{\tilde{\varepsilon}}\right) \tilde{v}_0^2 \tilde{\mathbf{d}}(1) \times \mathbf{B}'_0(\mathbf{x}, t + \Delta t/2) \\ & + \frac{\tilde{v}_0^2}{\tilde{\varepsilon}} \Delta\tilde{\mathbf{d}} \times \mathbf{B}'_0(\mathbf{x}, t + \Delta t/2) \end{aligned} \quad (10.43)$$

is the NS model of the scattered-field source current. Following the discussion of Section 7.4.3, the value of $\Delta\tilde{\mathbf{d}} \times \mathbf{B}'_0$ is very small and vanishes when $\hat{\mathbf{k}}_0$ is parallel to one of the coordinate axes; thus, we can neglect the last term in Eq. (10.43). Using Eq. (10.38b) and $d_t e^{-i\omega_0 t}/e^{-i\omega_0 t} = -2i \sin(\omega_0 \Delta t/2)$, the scattered-field source current becomes

$$\tilde{\mathbf{J}}_s = -2i \sin(\omega_0 \Delta t/2) \left(\frac{\tilde{\varepsilon} - 1}{\tilde{\varepsilon}} \right) \mathbf{E}_0. \quad (10.44)$$

For typical discretizations, little accuracy is lost by taking $\tilde{\mathbf{d}}(\sqrt{\varepsilon}) \rightarrow \tilde{\mathbf{d}}(1)$ in Eq. (10.42b).

10.4 Grid Representations for the Yee Algorithm

We now proceed to extend the fuzzy representation developed in Section 7.6 to the Yee algorithm. Figure 10.3 depicts an $h \times h$ pixel on the y - z plane

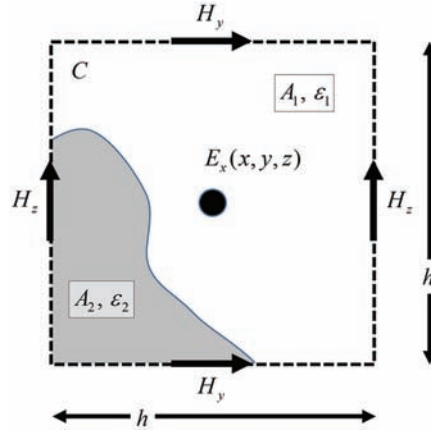


Figure 10.3 Layout to evaluate the effective value of ϵ at the position of E_x in the fuzzy model. Contour C lies on the y - z plane.

centered on grid point $\mathbf{x} = (x, y, z)$. The pixel is divided into two regions of different electrical permittivity: region 1 of area A_1 in which $\epsilon = \epsilon_1$, and region 2 of area A_2 in which $\epsilon = \epsilon_2$. A contour C on the y - z plane encloses the grid point (x, y, z) on which E_x is located.

From Ampere's law,

$$\oint_C \mathbf{H} \cdot d\boldsymbol{\ell} = \partial_t \int_{h \times h} \epsilon \mathbf{E} \cdot d\mathbf{s}, \quad (10.45)$$

where $d\mathbf{s} = \hat{\mathbf{x}} \, dy \, dz$ is a vector element of area, and $d\boldsymbol{\ell}$ is a vector element of length on the y - z plane. Using the Stokes theorem, the integral of $\mathbf{H}$ on C is equivalent to a surface integral over $h \times h$. Assuming $\mathbf{H}$ to vary slowly over $h \times h$, it follows that $\nabla \times \mathbf{H}(x, y', z', t) \cong \nabla \times \mathbf{H}(x, y, z, t)$, and the Stokes theorem gives

$$\begin{aligned} \oint_C \mathbf{H} \cdot d\boldsymbol{\ell} &= \hat{\mathbf{x}} \cdot \int_{h \times h} \nabla \times \mathbf{H}(x, y', z', t) \, dy' \, dz', \\ &\cong h^2 \hat{\mathbf{x}} \cdot [\nabla \times \mathbf{H}(x, y, t)]. \end{aligned} \quad (10.46)$$

Now, assuming that $\mathbf{E}$ (but not ϵ) varies slowly over $h \times h$, we remove it from the integral to obtain

$$\begin{aligned} \int_{h \times h} \epsilon \mathbf{E} \cdot d\mathbf{s} &= E_x(x, y, z, t) \int_{h \times h} dy' \, dz' \, \epsilon(x', y', z', t) \\ &= E_x(x, y, z, t) \, h^2 \langle \epsilon(x, y, z) \rangle_{y,z}, \end{aligned} \quad (10.47)$$

where $\langle \epsilon(x, y, z) \rangle_{y,z}$ is the average of $\epsilon(x, y, z)$ over the y - z plane.

Inserting Eqs. (10.46) and (10.47) into Eq. (10.45), we obtain

$$\langle \varepsilon(\mathbf{x}) \rangle_{y,z} \partial_t E_x(\mathbf{x}, t) = [\nabla \times \mathbf{H}(\mathbf{x}, t)]_x, \quad (10.48)$$

where $\mathbf{x} = (x, y, z)$. Thus, in the Yee algorithm, the local value of ε at a grid point is replaced by its average over a pixel centered on that grid point.

With reference to Fig. 10.3, we have $h^2 \langle \varepsilon(\mathbf{x}) \rangle_{y,z} = A_1 \varepsilon_1 + A_2 \varepsilon_2$, where $h^2 = A_1 + A_2$. Suppose that material 1 (white) of permittivity ε_1 is a substrate in which material 2 (gray) of permittivity ε_2 is immersed. Then the permittivity of material 2 relative to material 1 is $\varepsilon'_2 = \varepsilon_2/\varepsilon_1$, and it is easy to show that

$$\begin{aligned} \langle \varepsilon'_2 \rangle &= 1 + \frac{A_2}{h^2} (\varepsilon'_2 - 1) \\ &= 1 + \bar{S}(\varepsilon'_2 - 1), \end{aligned} \quad (10.49)$$

where $\bar{S}$ is the fuzzy inclusion function introduced in Section 7.6.

TE mode

Specifying the above developments to the TE mode, where $H_z = E_x = E_y = 0$, we obtain

$$\langle \varepsilon(\mathbf{x}) \rangle_{x,y} \partial_t E_z(\mathbf{x}, t) = \partial_x H_y(\mathbf{x}, t) - \partial_y H_x(\mathbf{x}, t). \quad (10.50)$$

TM mode

In the TM mode, where $H_x = H_y = E_z = 0$, Eq. (10.39) gives

$$\langle \varepsilon(\mathbf{x}) \rangle_y \partial_t E_x(\mathbf{x}, t) = \partial_y H_z(\mathbf{x}, t), \quad (10.51)$$

where $\mathbf{x} = (x, y)$. Here, $\langle \varepsilon(\mathbf{x}) \rangle_{y,z}$ is replaced by the line average

$$\langle \varepsilon(\mathbf{x}) \rangle_y = \frac{1}{h} \int_{y-h/2}^{y+h/2} dy' \varepsilon(x, y') \quad (10.52)$$

because all fields and parameters are presumed invariant along the z axis. Similarly, for E_x we have

$$\langle \varepsilon(\mathbf{x}) \rangle_x \partial_t E_y(\mathbf{x}, t) = -\partial_x H_z(\mathbf{x}, t). \quad (10.53)$$

The fuzzy method for the TM mode is not as accurate as that for the TE mode, and various improvements have been proposed. We recommend the methodology of Ref. 8, which takes into account the direction of the normal to the boundary within each subpixel. In this method, $\mathbf{E}$ is decomposed into normal and parallel components.

10.5 Algorithm Validation via Mie Scattering

In the Mie regime, in which the incident wavelength is about the same size as the scatterer, there are very few analytical solutions, even for such simple scatterer shapes as a square cylinder or cube. The analytical solutions that do exist can be used to verify the accuracy and correctness of numerical algorithms. Although there is no guarantee that an algorithm that correctly solves one problem will correctly solve another, this is the best we can do.

Let an infinite plane wave (vacuum wavelength $\lambda_0 = 8h$) of unit amplitude impinge from the negative x direction upon an infinite dielectric cylinder (radius $r = 0.75\lambda_0$, relative index of refraction $n_s = 1.7$). Taking $\mathbf{E}$ to be polarized in the y direction and the cylinder axis to be the z axis, the electromagnetic fields are in the TM mode ($H_x = H_y = E_z = 0$).

The scattered intensity of $\mathbf{E}_s = (E_x^s, E_y^s)$ is visualized in Fig. 10.4. Although the incident electric field is $\mathbf{E}_0 = \hat{y} E_{0,y}$, $\mathbf{E}_s$ contains a nonvanishing x component. The color scale is adjusted to show $|E_x^s|^2$, which is much smaller than $|E_y^s|^2$.

Figure 10.5 shows E_x^s and E_y^s as functions of scattering angle θ from the incident direction on a circular contour of radius $1.5\lambda_0$ about the cylinder center. The root-mean-square deviation δ from the analytic result of each FDTD calculation is noted on the graph.

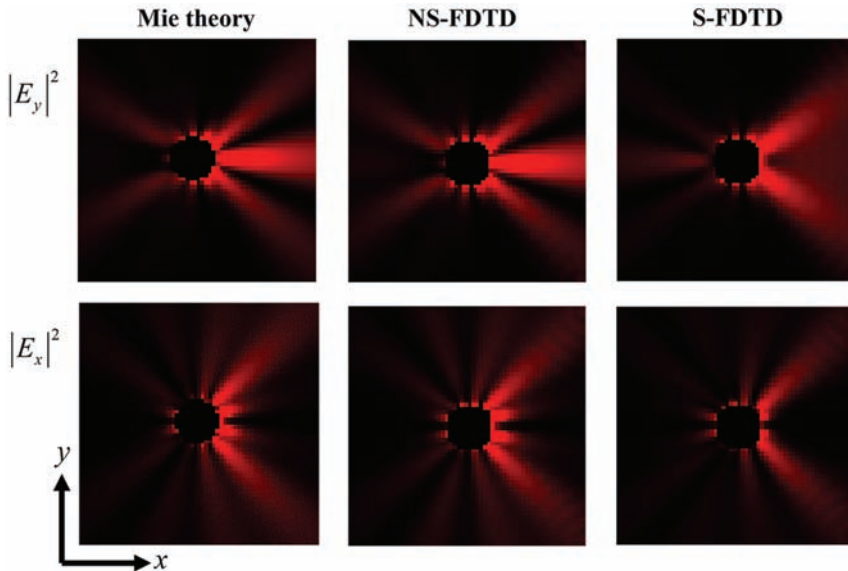


Figure 10.4 Visualization of $|E_x^s|^2$ and $|E_y^s|^2$ computed using Mie theory, the NS-Yee, and S-Yee algorithms. Intensity is visualized in shades of red; black = zero field or cylinder interior. The $|E_x^s|^2$ color scale is smaller than that of $|E_y^s|^2$.

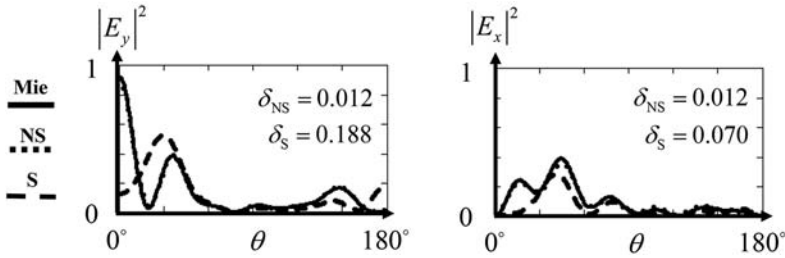


Figure 10.5 Scattered $|E_x|^2$ and $|E_y|^2$ as functions of scattering angle θ . The NS-Yee calculation (labeled “NS”) is almost indistinguishable from the analytic calculation (labeled “Mie”). Root mean square errors δ of each FDTD calculation are noted on the graph.

In the NS-Yee calculation, we took

$$J_{s,y}(\mathbf{x}, t) = -4\Theta_g(t) \sin^2(\omega_0 \Delta t/2) \left[\frac{\tilde{\epsilon}(\mathbf{x}) - 1}{\tilde{\epsilon}(\mathbf{x})} \right] \text{Re}[e^{i(k_0 \cdot \mathbf{x} - \omega_0 t)}], \quad (10.54)$$

where Θ_g turns on the source current over one wave period.

Important Topics of Chapter 10

- The S- and NS-Yee algorithm in two and three dimensions
- NS-Yee algorithm for the scattered field
- TE and TM modes
- The electric field in the TE mode computed using the wave equation for uniform magnetic permeability
- Structure models on the grid
- Mie scattering
- Mie resonances

Appendix 10.1 Mie Scattering off of a Cylinder in the TE Mode

In the TE mode, where $\mathbf{E} = \hat{\mathbf{z}}E_z$ and $\mathbf{H} = \hat{\mathbf{x}}H_x + \hat{\mathbf{y}}H_y$, Maxwell’s 3D equations reduce to their 2D form. Maxwell’s 2D equations further reduce to the wave equation in each region of constant ϵ and μ .

Putting $E_z \rightarrow \psi$, the wave equation to be solved is

$$\left(\partial_t^2 - \frac{v_0^2}{n^2} \nabla^2 \right) \psi(\mathbf{x}, t) = 0, \quad (\text{A10.1.1})$$

where $\mathbf{x} = (x, y)$, $n = n_s$ inside the cylinder; outside the cylinder, $n = 1$ and v_0 is the propagation velocity. The total field ψ is the sum of the incident field ψ_0 and the scattered field ψ_s ; thus, $\psi = \psi_0 + \psi_s$.

In FDTD calculations we take the initial scattered fields to be $\psi_s(\mathbf{x}, -\Delta t) = \psi_s(\mathbf{x}, 0) = 0$, but to develop the analytical solution, both the incident field (usually an infinite plane wave) and the scattered field are taken

to be present from $t \rightarrow -\infty$. Furthermore, we assume that $\psi_s \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$, and hence that $\psi \rightarrow \psi_0$ as $|\mathbf{x}| \rightarrow \infty$.

Solution of the wave equation in cylindrical coordinates

We now proceed to solve the wave equation for the case of an infinite plane wave incident upon an infinite cylinder. In cylindrical coordinates, $\mathbf{x} = (r\cos\theta, r\sin\theta, z)$. Taking ψ and n to be invariant with respect to z , $\partial_z\psi = 0$, the Laplacian reduces to

$$\nabla^2 = \partial_r^2 + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_\theta^2, \quad (\text{A10.1.2})$$

and the wave equation becomes

$$\left[\partial_t^2 - v^2 \left(\partial_r^2 + \frac{1}{r} \partial_r + \frac{1}{r^2} \partial_\theta^2 \right) \right] \psi(r, \theta, t) = 0, \quad (\text{A10.1.3})$$

where $v = v_0/n$. This equation can be solved by separation of variables. Postulating that $\psi(r, \theta, t) = X(r, \theta)T(t)$ and inserting it into $\partial_t^2\psi = v^2\nabla^2\psi$, we obtain

$$\frac{T''(t)}{T(t)} = v^2 \frac{\nabla^2 X(r, \theta)}{X(r, \theta)} = -\omega^2, \quad (\text{A10.1.4})$$

where ω is a real constant. Choosing $T''(t)/T(t) = -\omega^2$ (rather than $+\omega^2$) makes T an oscillatory function. Equation (A10.1.4) is equivalent to

$$T''(t) + \omega^2 T(t) = 0, \quad (\text{A10.1.5a})$$

$$(\nabla^2 + k^2)X(r, \theta) = 0. \quad (\text{A10.1.5b})$$

Equation (A10.1.5a) has two solutions: $T(t) = e^{\pm i\omega t}$. Since no initial conditions are specified, either one is acceptable, but we choose $T(t) = e^{-i\omega t}$. Equation (A10.1.5b) is the Helmholtz equation, and using Eq. (A10.1.2), its solution is found by postulating that $X(r, \theta) = R(r)\Theta(\theta)$ so that Eq. (A10.1.5b) becomes

$$r^2 \frac{R''(r)}{R(r)} + r \frac{R'(r)}{R(r)} + k^2 r^2 = -\frac{\Theta''(\theta)}{\Theta(\theta)} = m^2, \quad (\text{A10.1.6})$$

where m is a real constant. Equation (A10.1.6) is equivalent to

$$\Theta''(\theta) + m^2 \Theta(\theta) = 0, \quad (\text{A10.1.7a})$$

$$[r^2 \partial_r^2 + r \partial_r + (k^2 r^2 - m^2)]R(r) = 0. \quad (\text{A10.1.7b})$$

Because $(r, \theta + 2\pi)$ represents the same physical point as (r, θ) , we must have $\psi(r, \theta + 2m\pi) = \psi(r, \theta)$, so ψ must be periodic with period 2π . Therefore, we choose $m^2 \geq 0$, and m to be a positive or negative integer (including zero) so that

$$\Theta(\theta) = e^{im\theta}. \quad (\text{A10.1.8})$$

To solve for R it is convenient to define $\rho = kr$ and $P(\rho) = R(r)$ so that Eq. (A10.1.7b) becomes

$$[\rho^2 \partial_\rho^2 + \rho \partial_\rho + (\rho^2 - m^2)]P(\rho) = 0, \quad (\text{A10.1.9})$$

which is the standard form of the Bessel equation.

The Bessel equation has the solutions $Z_m(\rho) = J_m(\rho)$, $Y_m(\rho)$, $H_m^{(1)}(\rho)$, and $H_m^{(2)}(\rho)$; J_m is the Bessel function of the first kind, and Y_m is the Bessel function of the second kind (often called the Neumann function), which is linearly independent of J_m . $H_m^{(1)} = J_m + iY_m$ and $H_m^{(2)} = J_m - iY_m$ are called Hankel functions. All of these functions are sometimes collectively referred to as Bessel functions or cylinder functions.

Basis solutions of the wave equation in polar coordinates are thus

$$\psi(r, \theta, t) = e^{\pm i\omega t} Z_m(kr) e^{im\theta}. \quad (\text{A10.1.10})$$

Physical considerations and the properties of the cylinder functions now constrain the solution. The spatial part of $\psi(\mathbf{x}, t) = X(\mathbf{x})T(t)$ is a superposition of the form

$$X(r, \theta) = \sum_{m=-\infty}^{\infty} a_m Z_m(kr) e^{im\theta}, \quad (\text{A10.1.11})$$

where a_m are constants to be determined, and Z_m remain to be specified.

The incident field ψ_0 gives rise to an internal field (inside the cylinder) ψ_{in} , and a scattered field ψ_s outside that propagates outward from the cylinder boundary. The field outside the cylinder is thus $\psi_{\text{out}} = \psi_0 + \psi_s$, a superposition of the incident and scattered fields.⁹⁻¹¹

Note A10.1.1

The scattered field inside the cylinder could be defined as $\psi_{s,\text{in}} = \psi_{\text{in}} - \psi_0$.

To determine which of the solutions of Eq. (A10.1.9) are appropriate to construct ψ_s (outside the cylinder), let us examine the behavior of $Z_m(kr)$ for large r . For $\rho = kr \gg m^2 - 1/4$, it can be shown that

$$J_m(\rho) \rightarrow \sqrt{\frac{2}{\pi\rho}} \cos\left(\rho - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad (\text{A10.1.12})$$

$$Y_m(\rho) \rightarrow \sqrt{\frac{2}{\pi\rho}} \sin\left(\rho - \frac{m\pi}{2} - \frac{\pi}{4}\right). \quad (\text{A10.1.13})$$

Hence,

$$H_m^{(1)}(\rho) \rightarrow \sqrt{\frac{2}{\pi\rho}} \exp \left[i \left(\rho - \frac{m\pi}{2} - \frac{\pi}{4} \right) \right], \quad (\text{A10.1.14a})$$

$$H_m^{(2)}(\rho) \rightarrow \sqrt{\frac{2}{\pi\rho}} \exp \left[-i \left(\rho - \frac{m\pi}{2} - \frac{\pi}{4} \right) \right]. \quad (\text{A10.1.14b})$$

If we choose the solution of Eq. (A10.1.5a) to be $T(t) = e^{-i\omega t}$, then $e^{-i\omega t} H_m^{(1)}(kr) e^{im\theta}$ represents a wave propagating outward from the origin, while $e^{-i\omega t} H_m^{(2)}(kr) e^{im\theta}$ represents one converging onto it.

Following the notation of Ref. 11, ψ_s for $(r > a)$ is given by

$$\psi_s(r, \theta, t) = -e^{-i\omega t} \sum_{-\infty}^{\infty} i^m b_m H_m^{(1)}(k_0 r) e^{im\theta}, \quad (\text{A10.1.15})$$

where the expansion coefficients of ψ_s are taken to be $-i^m b_m$, $k_0 = \omega/\nu_0$ is the wavenumber outside the cylinder, and the constants b_m are to be determined.

To determine which solutions of Eq. (A10.1.9) are appropriate to construct the field inside the cylinder, we examine the behavior of $Z_m(kr)$ for a small kr . For $0 \leq \rho \ll \sqrt{m+1}$, it can be shown that

$$J_m(\rho) \rightarrow \frac{1}{m!} \left(\frac{\rho}{2} \right)^m, \quad (\text{A10.1.16})$$

$$Y_0(\rho) \rightarrow \frac{2}{\pi} \left[\ln \left(\frac{\rho}{2} \right) + \gamma \right], \quad (\text{A10.1.17a})$$

$$Y_m(\rho) \rightarrow -\frac{(m-1)!}{\pi} \left(\frac{2}{\rho} \right)^m \quad \text{for } m > 0, \quad (\text{A10.1.17b})$$

where $\gamma \cong 0.5772$ is the Euler–Mascheroni constant. Since Y_m and hence $H_m^{(1,2)}$ are singular at the origin, they are unsuitable solutions for ψ_{in} , leaving only J_m . Therefore, following Ref. 11, for $0 \leq r \leq a$, we take

$$\psi_{\text{in}}(r, \theta, t) = e^{-i\omega t} \sum_{m=-\infty}^{+\infty} i^m d_m J_m(n_s k_0 r) e^{im\theta}, \quad (\text{A10.1.18})$$

where d_m are to be determined.

Taking the incident field to an infinite plane wave propagating in the $+x$ direction, $\psi_0 = e^{i(k_0 \hat{\mathbf{x}} \cdot \mathbf{x} - \omega t)} = e^{i(k_0 r \cos \theta - \omega t)}$, where $\hat{\mathbf{x}}$ is a unit vector along the $+x$ axis, and k_0 is the wavenumber outside the cylinder. Since $e^{ip \cos \theta}$ is a periodic function of θ , it can be expanded in a Fourier series as

$$e^{i\rho \cos \theta} = \sum_{m=-\infty}^{+\infty} f_m(\rho) e^{im\theta}, \quad (\text{A10.1.19})$$

where

$$f_m(\rho) = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{i\rho \cos \theta} e^{-im\theta}. \quad (\text{A10.1.20})$$

f_m must be proportional to J_m (but not to Y_m or $H_m^{(1,2)}$, which are singular at the origin). Defining J_m by $J_m = i^{-m} f_m$, from Eq. (A10.1.20) we obtain

$$J_m(\rho) = \frac{i^{-m}}{2\pi} \int_0^{2\pi} d\theta e^{i\rho \cos \theta} e^{-im\theta}, \quad (\text{A10.1.21})$$

(see Note A10.1.2); thus, $f_m(\rho) = i^m J_m(\rho)$. Therefore,

$$\begin{aligned} e^{ik_0 \cos \theta} &= \sum_{m=-\infty}^{+\infty} i^m J_m(k_0 r) e^{im\theta} \\ &= J_0(k_0 r) + 2 \sum_{m=1}^{\infty} i^m J_m(k_0 r) \cos(m\theta), \end{aligned} \quad (\text{A10.1.22})$$

where we have used $J_{-m}(x) = (-1)^m J_m(x)$. Thus, the total field outside the cylinder is

$$\psi_{\text{out}}(r, \theta, t) = e^{-i\omega t} \sum_{m=-\infty}^{+\infty} i^m [J_m(k_0 r) - b_m H_m^{(1)}(k_0 r)] e^{im\theta}. \quad (\text{A10.1.23})$$

We can now determine the expansion coefficients b_m of ψ_{out} , and d_m of ψ_{in} by applying the boundary conditions of Eq. (7.4), requiring that the continuity of ψ across the dielectric boundary be equivalent to

$$\psi_{\text{in}}(r, \theta, t)|_{r=a} = \psi_{\text{out}}(r, \theta, t)|_{r=a}. \quad (\text{A10.1.24a})$$

Comparing coefficients of $e^{im\theta}$, we find that

$$d_m J_m(n_s k_0 a) = J_m(k_0 a) - b_m H_m^{(1)}(k_0 a). \quad (\text{A10.1.24b})$$

Next, requiring continuity of the normal derivative of ψ across the boundary, and again comparing coefficients of $e^{im\theta}$, we obtain

$$\partial_r \psi_{\text{in}}(r, \theta, t)|_{r=a} = \partial_r \psi_{\text{out}}(r, \theta, t)|_{r=a} \quad (\text{A10.1.25a})$$

$$\Rightarrow d_m n_s k_0 J'_m(n_s k_0 a) = k_0 J'_m(k_0 a) - b_m k_0 H_m^{(1)'}(k_0 a). \quad (\text{A10.1.25b})$$

Eliminating d_m from Eqs. (A10.1.24b) and (A10.1.25b), we find that

$$b_m = \frac{n_s J_m(k_0 a) J'_m(n_s k_0 a) - J_m(n_s k_0 a) J'_m(k_0 a)}{n_s H_m^{(1)'}(k_0 a) J'_m(n_s k_0 a) - J_m(n_s k_0 a) H_m^{(1)'}(k_0 a)}. \quad (\text{A10.1.26})$$

Now, knowing b_m , we find that

$$d_m = \frac{J_m(k_0 a) - b_m H_m^{(1)}(k_0 a)}{J_m(n_s k_0 a)}. \quad (\text{A10.1.27})$$

The expressions for the expansion coefficients can now be simplified by using the cylinder function properties

$$Z_{-m}(\rho) = (-1)^m Z_m(\rho), \quad (\text{A10.1.28})$$

$$\frac{d}{d\rho} Z_{-m}(\rho) = (-1)^m \frac{d}{d\rho} Z_m(\rho), \quad (\text{A10.1.29})$$

$$\frac{d}{d\rho} Z_m(\rho) = \frac{1}{2} [Z_{m-1}(\rho) - Z_{m+1}(\rho)], \quad (\text{A10.1.30})$$

$$Z_{m-1}(\rho) + Z_{m+1}(\rho) = \frac{2m}{\rho} Z_m(\rho). \quad (\text{A10.1.31})$$

From these it can be shown that

$$b_{-m} = b_m, \quad (\text{A10.1.32a})$$

$$d_{-m} = d_m. \quad (\text{A10.1.32b})$$

Summarizing our results, the scattered and interior fields are respectively given by

$$\psi_s(r, \theta, t) = -e^{-i\omega t} \left[b_0 H_0^{(1)}(k_0 r) + 2 \sum_{m=1}^{\infty} i^m b_m H_m^{(1)}(k_0 r) \cos(m\theta) \right], \quad (\text{A10.1.33})$$

$$\psi_{\text{in}}(r, \theta, t) = e^{-i\omega t} \left[d_0 J_0(n_s k_0 r) + 2 \sum_{m=1}^{\infty} i^m d_m J_m(n_s k_0 r) \cos(m\theta) \right]. \quad (\text{A10.1.34})$$

It can be proven that the summations of Eqs. (A10.1.33) and (A10.1.34) converge. These formulae also hold for complex n_s .

Note A10.1.2

From the definition given by Eq. (A10.1.21), using $i^{-n}e^{-in\theta} = e^{-in(\theta + \pi/2)}$ and $\cos(\theta - \pi/2) = \sin\theta$, changing variables and shifting the integration limits, we obtain the well-known formula

$$J_n(x) = \frac{1}{\pi} \int_0^\pi d\theta \cos(x \sin \theta - n\theta). \quad (\text{A10.1.35})$$

Note A10.1.3

There is no analytic solution to Mie scattering off of a square or rectangular cylinder because the fields cannot be expanded in a set of wave equation solutions (basis functions) that fulfill the boundary conditions.

Appendix 10.2 Mie Scattering off of a Cylinder in the TM Mode

In the TM mode, where $\mathbf{E} = \hat{\mathbf{x}}E_x + \hat{\mathbf{y}}E_y$ and $\mathbf{H} = \hat{\mathbf{z}}H_z$, Maxwell's equations reduce to the wave equation in each region of constant ϵ and μ . Since $\mathbf{H}$ has only one component H_z , and it is tangent to the cylinder boundary, we choose to solve for $\mathbf{E}$ in terms of H_z . Paralleling the developments in Appendix A10.1 (with E_z replaced by H_z), we postulate (using the notation of Ref. 11) that outside of the cylinder ($r \geq a = \text{cylinder radius}$), the scattered H_z field is given by

$$H_z^s(r, \theta, t) = -e^{-i\omega t} H_0 \sum_{m=-\infty}^{+\infty} i^m \alpha_m H_m^{(1)}(k_0 r) e^{im\theta}, \quad (\text{A10.2.1})$$

and inside the cylinder ($0 \leq r \leq a$) H_z is given by

$$H_z^{\text{in}}(r, \theta, t) = e^{-i\omega t} H_0 \sum_{m=-\infty}^{+\infty} i^m c_m J_m(n_s k_0 r) e^{im\theta}, \quad (\text{A10.2.2})$$

where H_0 is the amplitude of the incident magnetic field, and the constants α_m and c_m are determined by the boundary conditions on $\mathbf{E}$ and $\mathbf{H}$.

Since the electromagnetic fields tangential to the cylinder boundary must be continuous across it, we express $\mathbf{E}$ in terms of its radial and tangential components as $\mathbf{E} = E_r \hat{\mathbf{r}} + E_\theta \hat{\boldsymbol{\theta}}$, where $\hat{\mathbf{r}} = \hat{\mathbf{x}} \cos \theta + \hat{\mathbf{y}} \sin \theta$ and $\hat{\boldsymbol{\theta}} = -\hat{\mathbf{x}} \sin \theta + \hat{\mathbf{y}} \cos \theta$, and $E_r = \mathbf{E} \cdot \hat{\mathbf{r}}$ and $E_\theta = \mathbf{E} \cdot \hat{\boldsymbol{\theta}}$. In cylindrical coordinates, the curl of a vector field $\mathbf{V}$ is

$$\nabla \times \mathbf{V} = \hat{\mathbf{r}} \left(\frac{1}{r} \partial_\theta V_z - \partial_z V_\theta \right) + \hat{\boldsymbol{\theta}} (\partial_z V_r - \partial_r V) + \hat{\mathbf{z}} \frac{1}{r} [\partial_r (r V_\theta) - \partial_\theta V_r]. \quad (\text{A10.2.3})$$

In the TM mode,

$$\nabla \times \mathbf{H} = \hat{\mathbf{r}} \frac{1}{r} \partial_\theta H_z - \hat{\boldsymbol{\theta}} \partial_r H_z, \quad (\text{A10.2.4})$$

$$\nabla \times \mathbf{E} = \hat{\mathbf{z}} \frac{1}{r} [\partial_r (r E_\theta) - \partial_\theta E_r]. \quad (\text{A10.2.5})$$

With $e^{-i\omega t}$ time dependence, Maxwell's equation $\varepsilon \partial_t \mathbf{E} = \nabla \times \mathbf{H}$ becomes

$$i\varepsilon\omega E_r = \frac{-1}{r} \partial_\theta H_z, \quad (\text{A10.2.6a})$$

$$i\varepsilon\omega E_\theta = \partial_r H_z. \quad (\text{A10.2.6b})$$

The total electromagnetic field is $\mathbf{E} = \mathbf{E}^0 + \mathbf{E}^s$, $\mathbf{H} = \mathbf{H}^0 + \mathbf{H}^s$, where $\mathbf{E}^s$ and $\mathbf{H}^s$ are the scattered fields. Taking the incident electric field to be $\mathbf{E}^0 = \hat{\mathbf{y}} \psi_0$, where $\psi_0 = e^{i(k_0 \hat{\mathbf{x}} \cdot \mathbf{x} - \omega t)}$, the incident magnetic field from Eq. (10.32) is

$$\mathbf{H}^0 = \frac{\omega}{k_0} \hat{\mathbf{z}} \psi_0. \quad (\text{A10.2.7})$$

Thus, its amplitude is $H_0 = \omega/k_0$. Hence, from Eq. (A10.1.22),

$$H_z^0 = e^{-i\omega t} \frac{\omega}{k_0} \sum_{m=-\infty}^{+\infty} i^m J_m(k_0 r) e^{im\theta}. \quad (\text{A10.2.8})$$

From Eq. (A10.2.1), the total magnetic field outside of ($r \geq a$) the cylinder is

$$H_z^{\text{out}}(r, \theta, t) = e^{-i\omega t} \frac{\omega}{k_0} \left[\sum_{m=-\infty}^{+\infty} i^m J_m(k_0 r) e^{im\theta} - \sum_{m=-\infty}^{+\infty} i^m \alpha_m H_m^{(1)}(k_0 r) e^{im\theta} \right]. \quad (\text{A10.2.9})$$

Equating $H_z^{\text{out}}(a, \theta, t) = H_z^{\text{in}}(a, \theta, t)$, we obtain a relationship between α_m and c_m . To obtain a second relationship between α_m and c_m , we equate $E_\theta^{\text{out}}(a, \theta, t) = E_\theta^{\text{in}}(a, \theta, t)$. From Eq. (A10.2.6b), for $r \geq a$,

$$\begin{aligned}
 E_{\theta}^0 &= \frac{1}{i \varepsilon \omega} \partial_r H_z^0 \\
 &= e^{-i\omega t} \frac{1}{i} \sum_{m=-\infty}^{+\infty} i^m J'_m(k_0 r) e^{im\theta},
 \end{aligned} \tag{A10.2.10}$$

where $\partial_r J_m(k_0 r) = k_0 \partial_r J'_m(k_0 r)$ and $\varepsilon = 1$ outside the cylinder. Similarly,

$$E_{\theta}^s = i e^{-i\omega t} \sum_{m=-\infty}^{+\infty} i^m \alpha_m H_m^{(1)}(k_0 r) e^{im\theta}. \tag{A10.2.11}$$

Thus, the tangential electric field outside of the cylinder is $E_{\theta}^{\text{out}} = E_{\theta}^0 + E_{\theta}^s$, and

$$E_{\theta}^{\text{out}}(r, \theta, t) = i e^{-i\omega t} \left[\sum_{m=-\infty}^{+\infty} i^m \alpha_m H_m^{(1)}(k_0 r) e^{im\theta} - \sum_{m=-\infty}^{+\infty} i^m J'_m(k_0 r) e^{im\theta} \right]. \tag{A10.2.12}$$

Inside the cylinder, where $\varepsilon = n_s^2$ for $0 \leq r \leq a$, Eqs. (A10.2.6b) and (A10.2.2) give

$$E_{\theta}^{\text{in}}(r, \theta, t) = e^{-i\omega t} \frac{1}{i n_s} \sum_{m=-\infty}^{+\infty} i^m c_m J'_m(n_s k_0 r) e^{im\theta}. \tag{A10.2.13}$$

Finally, equating $E_{\theta}^{\text{out}}(a, \theta, t) = E_{\theta}^{\text{in}}(a, \theta, t)$, we obtain a second relationship connecting α_m with c_m . We then find that

$$\alpha_m = \frac{J_m(k_0 a) J'_m(n_s k_0 a) - n_s J_m(n_s k_0 a) J'_m(k_0 a)}{H_m^{(1)}(k_0 a) J'_m(n_s k_0 a) - n_s J_m(n_s k_0 a) H_m^{(1)}(k_0 a)}, \tag{A10.2.14}$$

$$c_m = \frac{J_m(k_0 a) - \alpha_m H_m^{(1)}(k_0 a)}{J_m(n_s k_0 a)}. \tag{A10.2.15}$$

α_m and c_m completely specify the electromagnetic field, and we can now derive its remaining components. From Maxwell's Eq. (A10.2.6b), we have

$$\begin{aligned}
 E_r^s &= \frac{i}{\omega r} \partial_{\theta} H_z^s \\
 &= \frac{1}{k_0 r} e^{-i\omega t} \sum_{m=-\infty}^{+\infty} i^m m \alpha_m H_m^{(1)}(k_0 r) e^{im\theta},
 \end{aligned} \tag{A10.2.16}$$

and

$$\begin{aligned}
 E_r^{\text{in}} &= \frac{i}{r\epsilon\omega} \partial_\theta H_z^{\text{in}} \\
 &= e^{-i\omega t} \frac{-1}{k_0 r n_s^2} \sum_{m=-\infty}^{+\infty} m i^m c_m J_m(n_s k_0 r) e^{im\theta}. \quad (\text{A10.2.17})
 \end{aligned}$$

From the cylinder function properties of Eqs. (A10.1.28) and (A10.1.32), it is easy to show that

$$\alpha_{-m} = (-1)^m \alpha_m, \quad (\text{A10.2.18a})$$

$$c_{-m} = (-1)^m c_m. \quad (\text{A10.2.18b})$$

We thus obtain simplified expressions suitable for computation:

$$E_r^{\text{s}} = e^{-i\omega t} \frac{2i}{k_0 r} \sum_{m=1}^{\infty} i^m m \alpha_m H_m^{(1)}(k_0 r) \sin(m\theta), \quad (\text{A10.2.19})$$

$$E_\theta = i e^{-i\omega t} \left[\alpha_0 H_0'^{(1)}(k_0 r) + 2 \sum_{m=1}^{\infty} i^m \alpha_m H_m'^{(1)}(k_0 r) \cos(m\theta) \right], \quad (\text{A10.2.20})$$

$$E_r^{\text{in}} = e^{-i\omega t} \frac{-2i}{n_s^2 k_0 r} \sum_{m=1}^{\infty} m i^m c_m J_m(n_s k_0 r) \sin(m\theta), \quad (\text{A10.2.21})$$

$$\begin{aligned}
 E_\theta^{\text{in}}(r, \theta, t) &= e^{-i\omega t} \frac{-i}{n_s} \left[c_0 J_0'(n_s k_0 r) + 2 \sum_{m=1}^{\infty} i^m c_m J_m'(n_s k_0 r) \cos(m\theta) \right]. \\
 &\quad (\text{A10.2.22})
 \end{aligned}$$

In FDTD calculations, because of the layout of the fields on the Yee grid, what we actually compute are E_x and E_y , which are given by

$$E_x = E_r \cos \theta - E_\theta \sin \theta, \quad (\text{A10.2.23})$$

$$E_y = E_r \sin \theta + E_\theta \cos \theta. \quad (\text{A10.2.24})$$

Appendix 10.3 Cylindrical Whispering Gallery Modes

A whispering gallery mode (WGM) is a resonance in which the fields are very strong in a few locations and weak elsewhere. Cylinders and spheres in the Mie regime support WGMs. In this section we derive the WGMs for infinite dielectric cylinders based on the discussions of Appendices 10.1 and 10.2.

TE resonance ($H_z = E_x = E_y = 0$) of a cylinder

A resonance occurs when one (or more) of the interior expansion coefficients d_m given by Eq. (A10.1.27) is large. Using the cylinder properties [Eqs. (A10.1.28–31)], d_m can be rewritten as

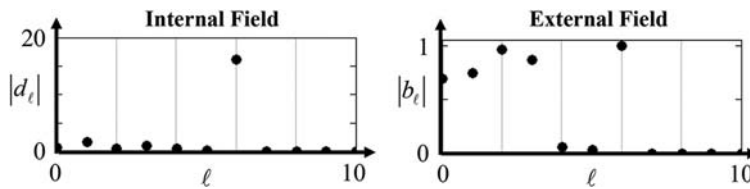


Figure A10.3.1 Mie expansion coefficients at a resonance; $k_0 a = \pi$ and $n_s = 2.745$.

$$d_m = \frac{J_{m-1}(k_0 a) H_m^{(1)}(k_0 a) - J_m(k_0 a) H_{m-1}^{(1)}(k_0 a)}{n_s J'_m(n_s k_0 a) H_m^{(1)}(k_0 a) - J_m(n_s k_0 a) H'_m{}^{(1)}(k_0 a)}. \quad (\text{A10.3.1})$$

The condition in which the denominator vanishes is

$$\frac{J_{m-1}(n_s k_0 a)}{J_m(n_s k_0 a)} = \frac{H_{m-1}^{(1)}(k_0 a)}{n_s H_m^{(1)}(k_0 a)}. \quad (\text{A10.3.2})$$

For example, at $k_0 a = \pi$ and $n_s = 2.745$, $|d_6|$ becomes large compared to the other expansion coefficients, as seen in Fig. A10.3.1.

For fixed $k_0 a$, the denominator of d_6 vanishes at $n_s \cong 2.745 - 0.001i$. A negative imaginary part of n_s is unphysical because it describes a material that produces energy (not an absorptive one), so an approximate resonance occurs at $n_s = 2.745$ (see Note A10.4.1). Some other parameters that produce TE resonances are listed in Table A10.3.1.

Table A10.3.1 Parameters producing TE resonances of a cylinder.

radius/wavelength (a/λ_0)	refractive index (n_s)	mode number (m)
0.50	2.745	6
0.75	2.310	8
1.00	2.717	10

Note A10.3.1

Referring to Eq. (4.50) in Section 4.2, in the complex wavenumber solution of the damped wave equation when the frequency is taken to be $\pm\omega$ ($\omega > 0$) and the absorption is taken to $\alpha > 0$, the imaginary part of the complex refractive index n_c is $\text{Im}(n_c) = \mp(\alpha/\omega)n$, where $n > 0$.

TM resonance ($H_x = H_y = E_z = 0$) of a cylinder

The condition for a TM resonance is that one or more of the internal expansion coefficients c_m given by Eq. (A10.2.15) is large. Again, using the cylinder function properties, we obtain

$$\frac{J_{m-2}(n_s k_0 a)}{J_{m-1}(n_s k_0 a)} = n_s \frac{H_{m-2}^{(1)}(k_0 a)}{H_{m-1}^{(1)}(k_0 a)} - \frac{(m-1)(n_s^2 - 1)}{n_s k_0 a}. \quad (\text{A10.3.3})$$

As is the case for the TE mode, the resonance condition [Eq. (A10.3.2)] cannot be exactly satisfied; nonetheless, one or more of the c_m values can be quite large. Table A10.3.2 lists some example TM resonance parameters.

Table A10.3.2 Parameters producing TM resonances of a cylinder.

radius/wavelength (a/λ_0)	refractive index (n_s)	mode number (m)
0.50	2.683	6
0.75	2.529	9
1.00	2.887	11

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Chapter 11

Example Applications of FDTD

The basic development of the FDTD methodology is now complete, and we now proceed to set up a few example problems. This and the remaining chapters are devoted to applications and design problems, and to the extension of the FDTD methodology to dispersive materials.

11.1 Beam Formation

In many problems we want to illuminate an object with a beam to compute transmission or scattering. For simplicity we consider two dimensions. In principle every point in the computational grid (except the boundary) can be a source point. If the Mur absorbing computational boundary is employed, source points should be at least three grid points away from the boundary.

Taking the source to be a line array as shown in Fig. 11.1, the amplitude and phase of the element located at y are $A(y)$ and $\phi(y)$ (real valued), respectively, and the complex amplitude is $A(y)e^{i\phi(y)}$. To minimize unwanted reflections from the computational boundaries, it is advisable that A vanish about one-half wavelength away from the boundary.

For angular frequency ω , the NS-FDTD wavenumber k is given by

$$\sin(kh/2) = \frac{\sin(\omega \Delta t/2)}{\tilde{v}}, \quad (11.1)$$

and the wavelength is given by $\lambda = 2\pi/k$, where, for numerical stability, $\tilde{v} \leq 0.80$ and 0.70 in two and three dimensions, respectively (see Appendices 7.1 and 7.2). The FDTD source term for an array positioned at x_0 along the x axis is

$$s(x, y, t) = \delta_{x, x_0} A(y) \Theta_g(t) \text{Re}(e^{i\phi(y)} e^{i\omega t}), \quad (11.2)$$

where

$$\Theta_g(t) = \Theta(t)(1 - e^{-t^2/\tau^2}) \quad (11.3)$$

is a turn-on function, and $\Theta(t)$ is the step function. In our experience, the results of FDTD calculations are not very sensitive to the value of τ , but we

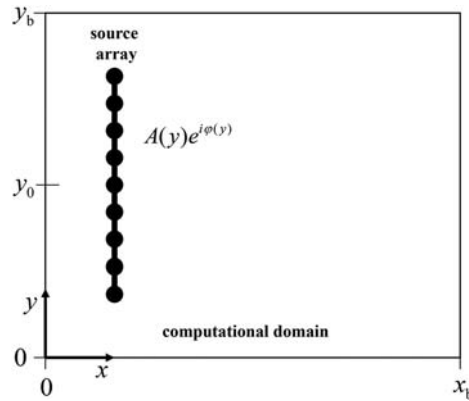


Figure 11.1 Linear source array in free space.

advise taking $\tau \geq T$, where the maximum wave period is T . Besides linear, other source array geometries are possible.

For the Yee algorithm, the source current is $J_{s,i}(x, y, t) = s(x, y, t)$, where $i = x$ or y .

11.1.1 Gaussian beam

We now define an approximation of a Gaussian beam suitable for FDTD calculations by taking $A = A_G$, where

$$\begin{aligned} A_G(y) &= \exp[-(y - y_0)^2 / \sigma^2] & \text{for } |y - y_0| \leq w, \\ &= 0 & \text{for } |y - y_0| > w. \end{aligned} \quad (11.4)$$

We advise taking $\sigma > \lambda$ and setting $w \geq 3\sigma$ such that A vanishes about $\lambda/2$ or more from the computational boundary. The beam can be steered by taking

$$\varphi(y) = (y - y_0)k \sin \theta, \quad (11.5)$$

so that it propagates at angle θ relative to the x axis, where k is given by Eq. (11.1).

An example beam is shown in Fig. 11.2. We used the following parameters in the NS-FDTD computation:

$$\lambda = 8h, 0 \leq x \leq 24\lambda, 0 \leq y \leq 24\lambda; \quad (11.6)$$

$$\sigma = 2\lambda, w = 3\sigma, \theta = 0, \tau = T. \quad (11.7)$$

The figure on the left in Fig. 11.2 is a visualization of the field intensity I , and the graph on the right compares $I(23\lambda, y)$ with $A(y)$ and illustrates the spreading of the beam. Figure 11.3 illustrates a steered beam.

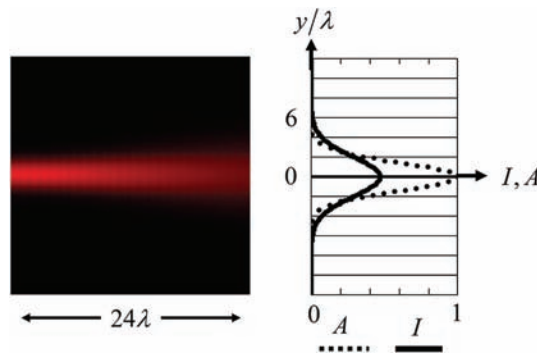


Figure 11.2 Gaussian beam with $A(0) = 1$, $\sigma = 2\lambda$, $w = 3\sigma$, and $\theta = 0$; I is the beam intensity at distance $x = 23\lambda$ from the source array. Solid line indicates beam spreading.

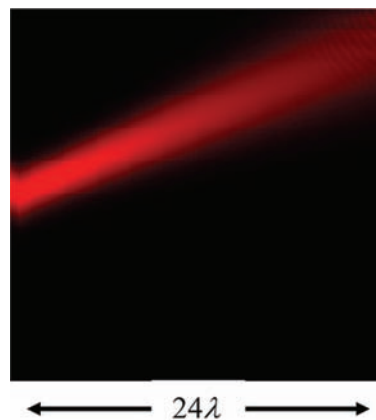


Figure 11.3 Gaussian beam with $A(0) = 1$, $\sigma = 2\lambda$, $w = 3\sigma$, and $\theta = \pi/8$.

Devil in the details

Technically, the phase factor φ in Eq. (11.5) is correct only for an infinite, uniformly weighted, linear source array, but even for Gaussian weighting and small values of λ/σ , the beam can be effectively steered, although there will be small variations in beam intensity, and the actual beam angle differs slightly from φ .

Now we insert a photonic crystal (pc), as shown in Fig. 11.4, into the computational domain. For example, taking $ar = 5$, $n_{pc} = 3$, and $n_{sub} = 1$, there is a bandgap at $\lambda/a = 2.53$ for an infinite photonic crystal.

Theoretical calculations of the bandgap assume an infinite plane wave, and in physical experiments, the beam width w is much larger than the lattice constant a of the photonic crystal. In FDTD calculations, we have found minimum transmission for $w/a \cong 3.7$ with $r = 1.2h$, in agreement with theory.

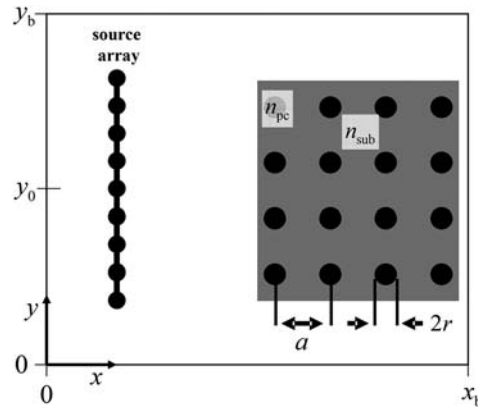


Figure 11.4 Photonic crystal illuminated by a source array: square lattice of circular cylinders (black) of refractive index n_{pc} embedded in a substrate (gray) of refractive index n_{sub} .

11.1.2 Bessel beam

A Bessel beam is defined by $A = A_B$, where $A_B(y) = J_0(|y - y_0|/\sigma)$. An approximate Bessel beam, suitable for the limited computational space of FDTD calculation, is given by

$$A_B(y) = J_0\left(\frac{|y - y_0|}{\sigma} Z_{0,1}\right) \quad \text{for } |y - y_0| \leq w = \frac{Z_{0,3}}{Z_{0,1}}\sigma, \\ = 0 \quad \text{for } |y - y_0| > w, \quad (11.8)$$

where $Z_{0,1} \cong 2.4048$, $Z_{0,2} \cong 5.5201$, and $Z_{0,3} \cong 8.6537$ are the first, second, and third zeros of $J_0(x)$, respectively. Taking $w = (Z_{0,2}/Z_{0,1})\sigma$ gives a narrower cutoff at the expense of more beam spreading, with fewer but wider and stronger side lobes.

Figure 11.5 shows an example Bessel beam. Although the Bessel beam spreading is less than that of the Gaussian beam, several side lobes accompany the main beam. The Bessel beam can also be steered.

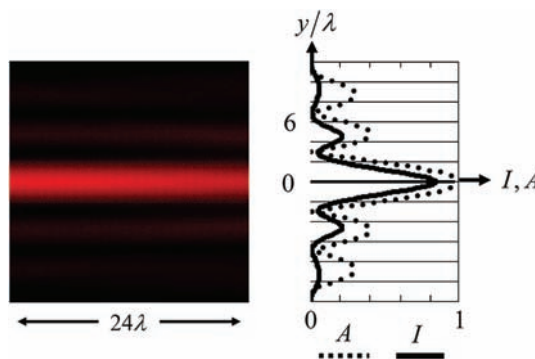


Figure 11.5 Bessel beam with $A(0) = 1$, $\sigma = 3\lambda$, $w = 3\sigma$, $w = (Z_{0,3}/Z_{0,1})\sigma$, and $\theta = 0$.



Figure 11.6 Airy–Gauss beam with $A(0) = 1$, $\sigma = 3\lambda$, $w = 4\lambda$, and $\theta = 0$.

11.1.3 Airy–Gauss beam

Beams that curve in free space can also be generated. A generic Airy beam is defined by

$$\varphi_A(y) = \exp \left[\left(\frac{y - y_0}{\sigma} \right)^3 \right] \quad (11.9)$$

with constant A . A form suitable for FDTD is an Airy beam with spatial Gaussian (or other modulation). In Fig. 11.6 we used $A_G(y)$ with $\sigma = 3\lambda$ and $w = 4\lambda$, and took

$$\varphi_A(y) = \exp \left[4\pi \left(\frac{y - y_0}{\sigma} \right)^3 \right]. \quad (11.10)$$

11.2 Whispering Gallery Modes and Devices

Resonators have many applications. Cylinders and spheres support what are called whispering gallery modes (WGMs), in which the field is highly concentrated in a few locations and vanishes elsewhere. In Appendix 10.3, we derived the conditions for the resonance of dielectric cylinders.

Correctly computing the electromagnetic field at resonance is a challenging problem. We have seen that the nonstandard (NS) FDTD algorithm gives a very accurate result; however, on resonance the dominant source of error is not the algorithm itself but the representation of the shape on the grid.

Consider, for example, an infinite dielectric cylinder in the TE mode illuminated by an infinite plane wave perpendicular to its axis. For cylinder radius $a = \lambda_0/2$ (λ_0 = incident wavelength) and refractive index $n_s = 2.7$, NS-FDTD gives a very accurate result for $h = \lambda_0/16$ ($h = \Delta x = \Delta y$), and the computation converges within about 5,000 time steps. On resonance ($a = \lambda_0/2$, $n_s = 2.745$), however, we need to take $h = \lambda_0/64$ to obtain an accurate result, and the calculation requires about 100,000 time steps to converge.

The very fine discretization is required because on resonance the field is very sensitive to the shape. The long convergence time is not merely a computational artifact, but reflects the physical fact that the electromagnetic field outside of the cylinder is weakly coupled to the inside. This is a consequence of reciprocity: on resonance, light is confined inside and only leaks out slowly; therefore, it couples in slowly. At $\lambda_0 = 640$ nm and $h = \lambda_0/64$, 100,000 time steps correspond to about $0.24 \mu\text{s}$ of real time. For the same computational parameters, standard (S) FDTD has very large errors.

Devil in the details

In the above example, if you didn't know that a resonance exists, you might think that taking $\lambda_0 = 16h$ and computing a few thousand time steps would yield an accurate calculation of the scattered field. On resonance, however, the error is dominated by the grid representation, and the light couples in very slowly so that many more time steps and a much finer grid are required.

In Ref. 1 we examined the errors in S- and NS-FDTD calculations of resonant scattering from dielectric cylinders. In both the TE ($\mathbf{E}$ parallel to the cylinder axis) and TM ($\mathbf{E}$ perpendicular to the cylinder axis) modes, fine grids are required to achieve reasonable accuracy, but the error is generally higher in the TM mode for the same discretization.

In the TE mode there is a resonance at $n_s = 2.31026$ and $a = 0.75\lambda_0$. Shifting the refractive index $n_s \rightarrow n'_s = 2.30826$ while maintaining the same cylinder radius, a fractional change of -0.09% causes a large change in the field, as seen in Figs. 11.7 and 11.8. Figure 11.9 shows how the Mie series expansion coefficients (see Chapter 10) are affected by a small shift in n_s . Thus, by

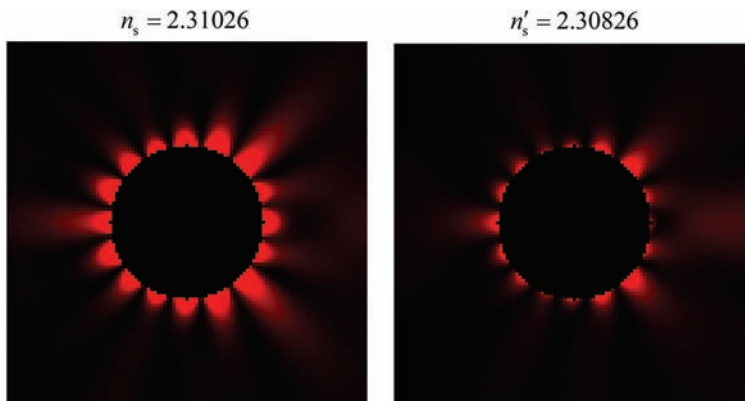


Figure 11.7 Scattered field intensity $|E_z^s|^2$ due to an infinite plane wave impinging on a resonant dielectric cylinder perpendicular to its axis. Computation uses Mie theory for the TE mode with $a = 0.75\lambda_0$ for $n_s = 2.31026$ (resonance), and $n_s = n'_s = 2.30826$ (off resonance). Visualization is outside the cylinder.

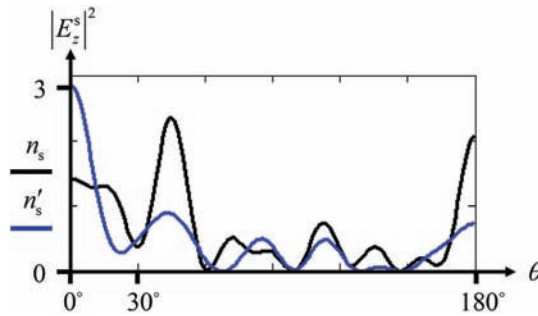


Figure 11.8 Scattered field intensity data of Fig. 11.7 plotted on a contour of radius $1.5 \lambda_0$ about the cylinder center; $a = 0.75 \lambda_0$ with $n_s = 2.31026$ (resonance), and $n_s = n'_s = 2.30826$ (off resonance).

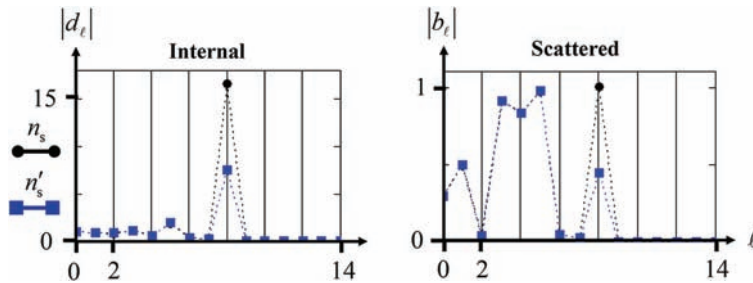


Figure 11.9 Effect of shifting the refractive index on the Mie expansion coefficients of the internal and scattered fields for a resonant dielectric cylinder; $a = 0.75 \lambda_0$, $n_s = 2.31026$ (resonance), and $n'_s = 2.30826$ (slightly off resonance). The greatest shift is in the $\ell = 8$ coefficient; other shifts are small.

modulating the refractive index, we can effect large changes in the coupling of light into and out of the resonator. The resonance is also very sensitive to changes in the size of the cylinder. This effect can be used to make a pressure sensor or a deformation sensor. The high sensitivity of the resonance can be exploited in a variety of applications, such as quantum computing.²

Next, keeping $n_s = 2.31026$ constant and shifting the radius $a = 0.75 \lambda_0 \rightarrow a' = 0.999a$, we again see a large change in the scattered field intensity, as seen in Fig. 11.10.

A source can be placed within the resonator to produce a field qualitatively similar to that shown in Fig. 11.7 (left). Since the light source is inside the resonator, the electromagnetic fields build up rapidly and converge after just a few thousand time steps ($\lambda_0 = 32h$, $n_s = 2.745$, TE mode). When the resonators are closely spaced, as shown in Figs. 11.11, the electromagnetic fields evanescently couple. Figure 11.12 depicts a wavelength separator using coupled WGM resonators.³

The resonance and the coupling are quite sensitive to the values of λ_0 , the refractive index, and the resonators' sizes and spacing. Thus, arrays of WGM

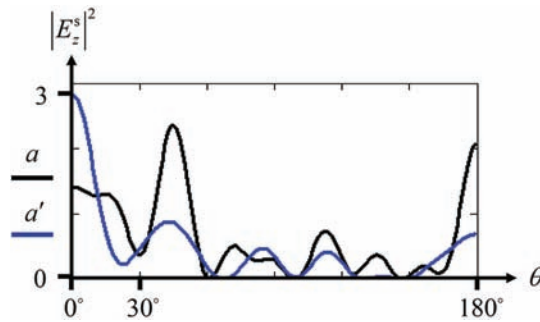


Figure 11.10 Scattered field intensity due to an infinite plane wave impinging on a resonant dielectric cylinder perpendicular to its axis. Computation uses Mie theory for the TE mode with $n_s = 2.31026$ for radius $a = 0.75\lambda_0$ (resonance) and radius $a' = 0.999a$ (off resonance); plotted on a contour of radius $1.5\lambda_0$ about the cylinder axis.

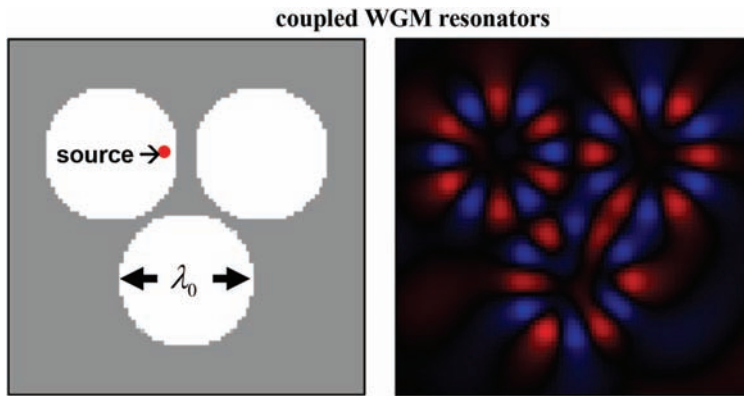


Figure 11.11 Evanescently coupled optical WGM resonators with $\lambda_0 = 32h$, $n_s = 2.745$, TE mode.

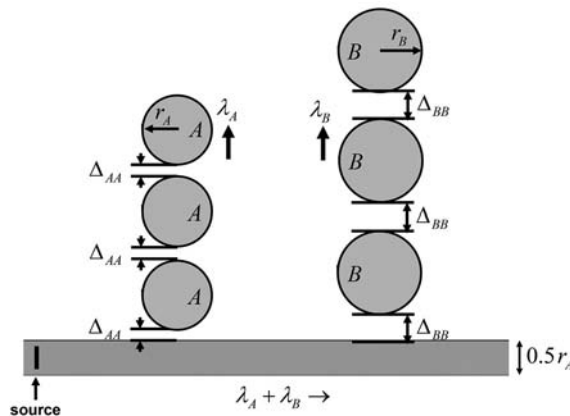


Figure 11.12 Wavelength separator. Evanescently coupled resonators extract signals from an optical waveguide. Resonators A and B resonate at wavelengths λ_A and λ_B , respectively.

resonators can be used as sensors to detect small changes and can be configured to separate multimode signals. The electromagnetic fields in the configurations of Figs. 11.11 and 11.12 cannot be calculated analytically.

References

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Chapter 12

FDTD for Dispersive Materials

Many nontransparent materials used in optics and optoelectronics devices show frequency-dependent complex electrical permittivity in the visible domain. The complex refractive index of bulk material is an important parameter that determines the optical behavior of a given material and in many cases any nanophotonic structure that might be fashioned from such a material. The complex refractive index for materials in the visible domain is given by the square root of the electrical permittivity [Eq. (8.36)]. The complex refractive index constitutes an important simulation parameter in optics and photonics. The imaginary parts of the refractive index and the electrical permittivity are associated with the absorption and the conductivity of the material, respectively. It is also important to understand that the implementation of FDTD depends on the actual relations among various components of the electric and magnetic fields, which in turn are determined by the nature of material properties. In this chapter we develop a simple dispersive algorithm that can be used when metal nanostructures need to be simulated in the visible domain.

Topics

- Material dispersion
- Monochromatic recursive convolution FDTD
- Computing extinction and scattering cross-sections from FDTD

12.1 Material Dispersion and Dispersive FDTD

The electrical permittivity of most naturally available materials is a complex quantity of the form $\tilde{\epsilon} = \tilde{\epsilon}_r + i\tilde{\epsilon}_i$, where $\tilde{\epsilon}_r$ and $\tilde{\epsilon}_i$ are the real and imaginary parts, respectively. In the Lorentz model,¹ the permittivity in the frequency domain is given by

$$\tilde{\epsilon} = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega(\omega + i\nu_c)}, \quad (12.1)$$

where ω is the angular frequency of the light, ω_p is the plasma frequency, ω_0 is a natural oscillation frequency, and ν_c is the collision frequency.

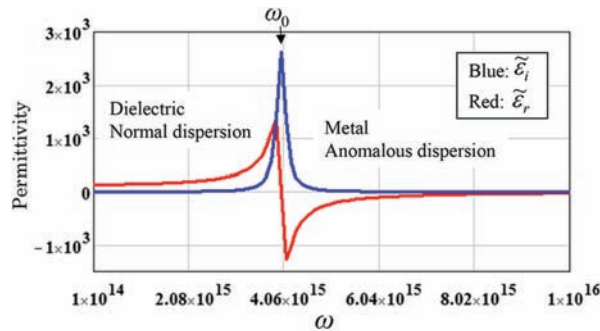


Figure 12.1 Real and imaginary parts of permittivity ($\tilde{\epsilon}_r$ and $\tilde{\epsilon}_i$, respectively) as a function of angular frequency ω .

Here, $\tilde{f}(\omega) = \mathcal{F}[f(t)]$, where $\mathcal{F}$ denotes the Fourier transform (see Section 8.4.1). Separating the real and imaginary parts of $\tilde{\epsilon}$ in Eq. (12.1), we plot them as functions of ω in Fig. (12.1). The real and imaginary parts of permittivity are related to each other by the Kramers–Kronig relations given in Section 8.5, so if we know one, we know the other.

To plot Fig. 12.1, we used $\omega_p = 4.6 \times 10^{16}/\text{s}$ and $\omega_0 = 4.06 \times 10^{15}/\text{s}$. Values of ω_p and ω_0 are different for different materials. For mostly transparent dielectric materials, the electrical permittivity displays normal dispersion behavior characterized by $\tilde{\epsilon}_r > 0$ and $\tilde{\epsilon}_r > \tilde{\epsilon}_i$. This behavior is shown in the $\omega < \omega_0$ range in Fig. (12.1). For most metals in the visible domain of the electromagnetic spectrum (380- to 780-nm wavelength range), the dependence of $\tilde{\epsilon}$ on ω can be described by the anomalous dispersion behavior shown in the $\omega_0 < \omega < \omega_p$ range in Fig. (12.1). The anomalous dispersion regime is characterized by strong frequency dependence of $\tilde{\epsilon}$, $\tilde{\epsilon}_r \leq 0$, and $\tilde{\epsilon}_r < \tilde{\epsilon}_i$.

The FDTD algorithm described in previous chapters that works so well for dielectric materials becomes numerically unstable in this regime. Special-purpose FDTD algorithms, such as the recursive convolution (RC) FDTD,^{1,2} the auxiliary differential equation (ADE) FDTD,^{3–5} the frequency-dependent Z transform method,⁶ the piecewise linear recursive convolution (PLRC) method,⁷ etc., have been developed to compute propagation in dispersive and nonlinear, active, gain,^{8,9} or anisotropic media¹⁰ in the visible domain. In theory, some of these dispersive FDTD algorithms are preferable to the ordinary FDTD method that was discussed in previous chapters, mainly because these algorithms can be employed with a wide range of materials in various frequency ranges. However, the actual implementation of such algorithms over a broad band of frequencies for all materials is quite tricky. Part of the problem is that the material permittivities over a broad range of frequencies do not perfectly fit any given analytical model. Permittivity models such as multipole Drude–Lorentz¹¹ and fancier ones such as the critical point model^{12,13} were variously employed. This reveals the difficulty that one

faces when choosing an appropriate permittivity model for a given material. A somewhat simplistic way to circumvent this issue would be to use a monochromatic implementation of the dispersive algorithms.

We have developed a monochromatic version of the RC-FDTD method (MRC-FDTD).^{14,15} The stability of the MRC-FDTD algorithm in the anomalous dispersion regime is ensured by recursively implementing a convolution operation performed on an analytical model of electrical permittivity.

12.1.1 Recursive convolution FDTD and its monochromatic cousin

To effectively implement RC-FDTD, an analytical model of dispersive permittivity is needed. Conventionally, RC-FDTD is implemented for pulsed-light sources. An input pulse is propagated into the material, and amplitudes of the Fourier components of the input and transmitted pulses are compared using a discrete Fourier transform (DFT).

This requires that the analytical model of permittivity closely fit the handbook (experimentally determined) permittivities over the broad band of frequencies contained in the input pulse. However, this is not an easy task. It turns out that the choice of a particular analytical model depends on the metal that is being simulated. Each simulated metal requires a carefully chosen analytical model that fits the handbook permittivity values as closely as possible over a very broad band of frequencies. No model does this perfectly. In addition, as we have seen in Section 6.5.4, large errors can result in the DFT calculation of the spectrum.

In this section, we discuss our implementation of the monochromatic RC-FDTD (MRC-FDTD). This algorithm uses the first-order Drude model² to evaluate the convolution operation needed to make FDTD stable for metals, for which the real part of permittivity is negative. In the first-order Drude model,² $\tilde{\epsilon}(\omega)$ is given by

$$\tilde{\epsilon}(\omega) = 1 + \frac{\omega_p^2}{\omega(i\nu_c - \omega)}, \quad (12.2)$$

where ω_p is the plasma frequency, and ν_c is the collision frequency.

Unlike conventional RC-FDTD, in the MRC-FDTD scheme, the Drude parameters are computed at each wavelength of the incident light using the corresponding handbook value of permittivity. Hence, MRC-FDTD allows us to use handbook permittivity values at all wavelengths of interest instead of often-erroneous fit values. Another advantage of the monochromatic scheme is that it allows one to use the same permittivity model to simulate any material displaying anomalous dispersion behavior in a specified frequency (wavelength) range.

To show the difference between our MRC-FDTD and the broadband conventional RC-FDTD implemented with a first-order Drude model of

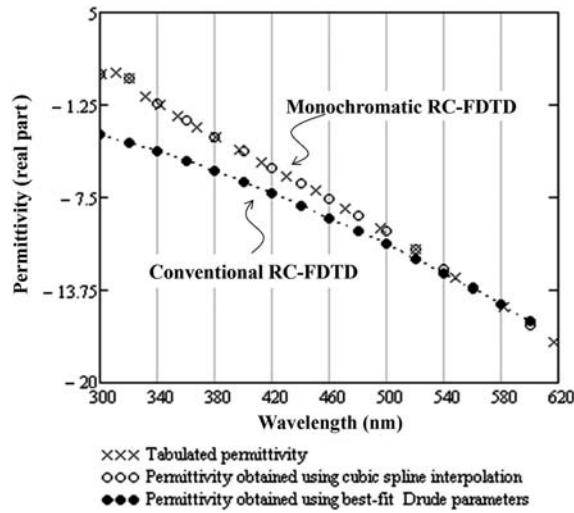


Figure 12.2 Comparison of wavelength spectra of three sets of the real part of permittivity: (1) tabulated handbook values based on experiment, (2) cubic spline interpolation of the tabulated permittivities, and (3) permittivity values derived from a first-order Drude dispersion model using a set of best-fit Drude parameters.

permittivity, in Fig. 12.2 we plot the handbook permittivity values for silver¹⁶ using a cubic spline interpolation of the handbook permittivity values versus the permittivity values obtained using the first-order Drude dispersion model with the best-fit Drude parameters. The cubic spline interpolation of the handbook permittivity values is carried out to determine the permittivity value at arbitrary wavelengths (e.g., 380 nm) that do not correspond to the energy values specified in the material handbook. The figure shows that the permittivity values generated using the first-order Drude dispersion model with the best-fit Drude parameters can be quite different from those found by interpolating the handbook permittivity values.

The values of the best-fit Drude parameters ($\hat{\omega}_p$ and $\hat{\nu}_c$) were determined by fitting the first-order Drude model to the handbook permittivities over a broad range of frequencies spanning the entire visible domain. For this purpose, we used a genetic-algorithm (GA)-based optimization scheme.¹⁷ The best-fit $\hat{\omega}_p$ and $\hat{\nu}_c$ are obtained by minimizing a merit function given by

$$\phi = \frac{1}{N} \sqrt{\sum_{j=1}^N (\tilde{\epsilon}_{r,j} - \bar{\epsilon}_{r,j})^2 + \sum_{j=1}^N (\tilde{\epsilon}_{i,j} - \bar{\epsilon}_{i,j})^2}, \quad (12.3)$$

where N is the total number of frequency points, and $\bar{\epsilon}_{r,j}$ and $\bar{\epsilon}_{i,j}$ are, respectively, the real and imaginary parts of the handbook permittivity value at the j^{th} frequency ω_j . $\tilde{\epsilon}_{r,j}$ and $\tilde{\epsilon}_{i,j}$ are obtained from the first-order Drude

model [Eq. (12.2)] after separating the real and imaginary parts. Hence, $\tilde{\epsilon}_{r,j}$ and $\tilde{\epsilon}_{i,j}$ are given by

$$\tilde{\epsilon}_{r,j} = 1 - \frac{\omega_p^2}{\nu_c^2 + \omega_j^2}, \quad (12.4)$$

$$\tilde{\epsilon}_{i,j} = -\frac{\omega_p^2 \nu_c}{(\nu_c^2 + \omega_j^2) \omega_j}. \quad (12.5)$$

GA is a stochastic intelligent search method. In our implementation, the algorithm generates a random population of chromosomes and mimics a biological evolution process through a given number of generations. The evolution process is facilitated by the combination of a tournament selection scheme and a uniform crossover scheme. The GA parameters chosen are: population size of chromosomes = 500, number of generations = 100, tournament size = 5, tournament probability = 0.8, crossover probability = 0.8, and mutation probability = 0.01. With these settings, the best-fit Drude parameters for silver are $\hat{\omega}_p = 1.288 \times 10^{16} \text{ s}^{-1}$ and $\hat{\nu}_c = 6.4713 \times 10^{13} \text{ s}^{-1}$.

The MRC-FDTD is seen to work well with most metals, such as aluminium, silver, and gold, in the visible domain. For most metals, handbook permittivities indicate that the zero reversal of permittivity seen at $\omega = \omega_0$ (Fig. 12.1) occurs at wavelengths much shorter than 400 nm, or the smallest wavelength of interest—an important point for the first-order Drude model to work efficiently. This is because the first-order Drude permittivity model [Eq. (12.2)] does not include ω_0 and therefore cannot be used to model the zero reversal or the normal dispersion regime of permittivity. On the other hand, for commonly used metals in photonics in the visible domain, MRC-FDTD with the first-order Drude model is good for all practical purposes. Consequently, the MRC-FDTD approach makes it unnecessary to choose an analytical model of permittivity suitable for the metal being simulated.

In the following sections, we describe the implementation of MRC-FDTD in two and three dimensions. 2D computations require less computational resource than 3D computations and can yield meaningful results for 2D structures that are practically invariant in the third dimension.

As was shown in Section 10.2.2, if the magnetic permeability μ remains spatially constant, Maxwell's equations in the TE mode ($H_z = E_x = E_y = 0$) reduce to the wave equation in E_z . Thus, in the TE mode it is not necessary to compute any component of the magnetic field (assuming μ to be positive, constant, and nondispersive), greatly reducing the computational cost. We introduced a new formulation of RC-FDTD for the wave equation.¹⁴ In the TM mode or in three dimensions, Maxwell's curl equations are implemented in the MRC-FDTD framework.

2D FDTD can be used to simulate 3D structures that are invariant in one dimension. In most practical problems involving metal nanoparticles or nanostructures, useful 3D computations are still out of reach due to extraordinary requirements of memory and computation time. Some of these problems can, however, be solved in two dimensions, yielding results that might be of great practical and physical significance.

12.2 Mathematical Description of MRC-FDTD

Let us now develop a solution to Maxwell's equations in the form

$$\mu \partial_t \mathbf{H}(\mathbf{x}, t) = -\nabla \times \mathbf{E}(\mathbf{x}, t), \quad (12.6a)$$

$$\partial_t \mathbf{D}(\mathbf{x}, t) = \nabla \times \mathbf{H}(\mathbf{x}, t), \quad (12.6b)$$

where μ , the magnetic permeability, is constant, but ε is dispersive so that $\mathbf{D} \neq \varepsilon \mathbf{E}$ in the time domain. Assuming a linear medium, $\tilde{\mathbf{D}}(\mathbf{x}, \omega) = \tilde{\varepsilon}(\mathbf{x}, \omega) \tilde{\mathbf{E}}(\mathbf{x}, \omega)$ (see Section 8.4). Applying the convolution theorem [Eq. (A8.1.5)], and assuming that the electric field is to be switched on at $t = 0$, we have²

$$\begin{aligned} \mathbf{D}(t) &= \int_0^t \varepsilon(t') \mathbf{E}(t - t') dt' \\ &= \varepsilon_0 \mathbf{E}(t) + \int_0^t dt' \mathbf{E}(t') \chi(t - t'), \end{aligned} \quad (12.7)$$

where $\chi = \varepsilon - \varepsilon_0$ is the electric susceptibility [see Eq. (8.74)]. The $\mathbf{x}$ dependence is dropped for notational brevity.

We now proceed to develop the recursion convolution (RC) FDTD algorithm to solve Maxwell's equations [Eq. (12.6) together with Eq. (12.7)] in the time domain. Discretizing time by $t = \tau \Delta t$ ($\tau = 0, 1, 2, \dots$), we define $f^\tau = f(\tau \Delta t)$. For $0 \leq t'' \leq t - \Delta t$, and if $\Delta t \ll 2\pi/\omega$,

$$\int_{t''}^{t''+\Delta t} dt' \mathbf{E}(t - t') \chi(t') \cong \mathbf{E}(t - t'') \int_{t''}^{t''+\Delta t} dt' \chi(t'). \quad (12.8)$$

Defining $\chi^\tau = \int_{\tau \Delta t}^{(\tau+1) \Delta t} dt \chi(t)$,

$$\int_0^t dt' \mathbf{E}(t - t') \chi(t') \cong \sum_{\tau'=0}^{\tau-1} \mathbf{E}^{\tau-\tau'} \chi^{\tau'}. \quad (12.9)$$

Defining

$$\Psi^\tau = \sum_{\tau'=0}^{\tau-1} \mathbf{E}^{\tau-\tau'} \chi^{\tau'}, \quad (12.10)$$

Eq. (12.7) becomes

$$\mathbf{D}^\tau = \varepsilon_0 \mathbf{E}^\tau + \Psi^\tau. \quad (12.11)$$

We now take the difference

$$\mathbf{D}^{\tau+1} - \mathbf{D}^\tau = \varepsilon_0 (\mathbf{E}^{\tau+1} - \mathbf{E}^\tau) + \Delta \Psi^\tau, \quad (12.12)$$

where $\Delta \Psi^\tau = \Psi^{\tau+1} - \Psi^\tau$. Using $\partial_t \mathbf{D}|_{t+\Delta t/2} \cong (\mathbf{D}^{\tau+1} - \mathbf{D}^\tau)/\Delta t$, and solving for $\mathbf{E}^{\tau+1}$, the Yee algorithm takes the form

$$\mathbf{H}^{\tau+1/2} = \mathbf{H}^{\tau-1/2} - \frac{1}{\mu} \frac{\Delta t}{h} \mathbf{d} \times \mathbf{E}^\tau, \quad (12.13a)$$

$$\mathbf{E}^{\tau+1} = \mathbf{E}^\tau + \left(\frac{\Delta t}{\varepsilon_0 h} \mathbf{d} \times \mathbf{H}^{\tau+1/2} - \frac{1}{\varepsilon_0} \Delta \Psi^\tau \right). \quad (12.13b)$$

A third equation is now required to update $\Delta \Psi^\tau$, and for this purpose a model of the dispersion is needed.

Since Ψ^τ is vector quantity and contains the entire time history of the electric field, in a practical computation, it demands a very large amount of memory that increases with each step of the iteration. This load can be reduced if we can update Ψ^τ recursively.

In the first-order Drude model of Eq. (12.2), $\tilde{\chi}(\omega) = \omega_p^2 / \omega(iv_c - \omega)$. Taking the inverse Fourier transform, $\chi(t) = \mathbf{F}^{-1}[\tilde{\chi}(\omega)]$, we obtain

$$\begin{aligned} \chi(t) &= 0 & \text{for } t \leq 0, \\ &= \frac{\omega_p^2}{v_c} (1 - e^{-v_c t}) & \text{for } t > 0. \end{aligned} \quad (12.14)$$

Devil in the details

We take the time dependence of the electromagnetic fields to be $e^{+i\omega t}$, but if it is taken to be $e^{-i\omega t}$, the permittivity is given by the complex conjugate of Eq. (12.2), and $\tilde{\chi}(\omega) = -\omega_p^2 / \omega(iv_c + \omega)$.

Inserting Eq. (12.14) into the definition of χ^τ , we find that

$$\chi^\tau = \frac{\omega_p^2}{v_c^2} \left[v_c \Delta t - e^{-v_c \tau \Delta t} (1 - e^{-v_c \Delta t}) \right]; \quad (12.15)$$

hence, $\Delta\chi^\tau = \chi^{\tau+1} - \chi^\tau$ is

$$\Delta\chi^\tau = -\frac{\omega_p^2}{v_c^2}(e^{-v_c\Delta t} - 1)e^{-v_c\tau\Delta t}. \quad (12.16)$$

Defining

$$c_1 = \frac{\omega_p^2\Delta t}{v_c}(1 - e^{-v_c\Delta t}), \quad (12.17a)$$

$$c_2 = e^{-v_c\Delta t}, \quad (12.17b)$$

we find that

$$\chi^{\tau+1} = c_1 + c_2\chi^\tau. \quad (12.18)$$

Thus, $\chi^1 = c_1 + c_2\chi^0$, $\chi^2 = c_1 + c_1c_2 + c_2^2\chi^0, \dots$; hence,

$$\chi^\tau = c_1\left(\frac{1 - c_2^\tau}{1 - c_2}\right) + c_2^\tau\chi^0. \quad (12.19)$$

Using this model, let us now proceed to evaluate Ψ^τ . Using

$$\Delta\Psi^\tau = \chi^0(\mathbf{E}^{\tau+1} - \mathbf{E}^\tau) + \sum_{\tau'=1}^{\tau} \mathbf{E}^{\tau+1-\tau'}\chi^{\tau'} - \sum_{\tau'=1}^{\tau-1} \mathbf{E}^{\tau-\tau'}\chi^{\tau'}, \quad (12.20)$$

and $\chi^\tau = c_1 + c_2\chi^{\tau-1}$,

$$\begin{aligned} \sum_{\tau'=1}^{\tau} \mathbf{E}^{\tau+1-\tau'}\chi^{\tau'} - \sum_{\tau'=1}^{\tau-1} \mathbf{E}^{\tau-\tau'}\chi^{\tau'} &= c_1\left(\sum_{\tau'=1}^{\tau} \mathbf{E}^{\tau+1-\tau'} - \sum_{\tau'=1}^{\tau-1} \mathbf{E}^{\tau-\tau'}\right) \\ &\quad + c_2\left(\sum_{\tau'=1}^{\tau} \mathbf{E}^{\tau+1-\tau'}\chi^{\tau'-1} - \sum_{\tau'=1}^{\tau-1} \mathbf{E}^{\tau-\tau'}\chi^{\tau'-1}\right) \\ &= c_1E^\tau + c_2\left(\sum_{\tau''=0}^{\tau-1} \mathbf{E}^{\tau-\tau''}\chi^{\tau''}\right. \\ &\quad \left.- \sum_{\tau''=0}^{\tau-2} \mathbf{E}^{\tau-1-\tau''}\chi^{\tau''}\right). \end{aligned} \quad (12.21a)$$

The second term on the right side of Eq. (12.21a) is obtained by the substitution $\tau'' \rightarrow \tau' - 1$. Since $\chi^0 = 0$ (see Note 12.1), the summations in the second term above can be extended from $\tau'' = 1$ instead of $\tau'' = 0$. With these simplifications, we finally obtain

$$\sum_{\tau'=1}^{\tau} \mathbf{E}^{\tau+1-\tau'} \chi^{\tau'} - \sum_{\tau'=1}^{\tau-1} \mathbf{E}^{\tau-\tau'} \chi^{\tau'} = c_1 \mathbf{E}^{\tau} + c_2 \Delta \Psi^{\tau-1}. \quad (12.21b)$$

Hence, from Eq. (12.20), we find that

$$\Delta \Psi^{\tau} = \chi^0 (\mathbf{E}^{\tau+1} - \mathbf{E}^{\tau}) + c_1 \mathbf{E}^{\tau} + c_2 \Delta \Psi^{\tau-1}, \quad (12.22a)$$

or

$$\Psi^{\tau+1} - \Psi^{\tau} = \chi^0 (\mathbf{E}^{\tau+1} - \mathbf{E}^{\tau}) + c_1 \mathbf{E}^{\tau} + c_2 (\Psi^{\tau} - \Psi^{\tau-1}). \quad (12.22b)$$

We can now recursively update Ψ . Assuming that all electromagnetic fields vanish for $t \leq 0$, from definition Eq. (12.10), we find that $\Psi^0 = 0$ and $\Psi^1 = \chi^0 \mathbf{E}^1 = 0$.

Note 12.1

By definition, from Eq. (12.14),

$$\chi^{-1} = 0, \text{ and } \chi^0 = 0. \quad (12.23)$$

From Eqs. (12.22a) and (12.23), we now obtain the update

$$\Delta \Psi^{\tau+1} = c_1 \mathbf{E}^{\tau+1} + c_2 \Delta \Psi^{\tau}. \quad (12.24)$$

We can now construct a usable form of the Yee algorithm that includes anomalous dispersion. We refer to this form of FDTD as the MRC algorithm, which is given by

$$\mathbf{H}^{\tau+1/2} = \mathbf{H}^{\tau-1/2} - \frac{1}{\mu} \frac{\Delta t}{h} \mathbf{d} \times \mathbf{E}^{\tau}, \quad (12.25a)$$

$$\mathbf{E}^{\tau+1} = \mathbf{E}^{\tau} + \frac{\Delta t}{\varepsilon_0 h} \mathbf{d} \times \mathbf{H}^{\tau+1/2} - \frac{1}{\varepsilon_0} \Delta \Psi^{\tau}, \quad (12.25b)$$

$$\Delta \Psi^{\tau+1} = c_1 \mathbf{E}^{\tau+1} + c_2 \Delta \Psi^{\tau}. \quad (12.25c)$$

The MRC algorithm can be iterated with the initialization $\mathbf{H}^{-1/2} = \mathbf{E}^0 = \Delta \Psi^0 = 0$. RC-FDTD derives its name from the use of recursion to evaluate $\Psi^{\tau+1}$ without the need to save all of the intermediate steps. It is sufficient to know only c_1 and c_2 . Including Ψ , there are nine field components.

As with the ordinary (dispersionless) Yee algorithm, there is more than one way to lay out the fields on the grid. Our choice is shown in Fig. 12.3. Defining the time difference operator using a forward difference formula, we find that $d_{\tau}^t f^{\tau} = f^{\tau+1} - f^{\tau}$. The partial space difference operators

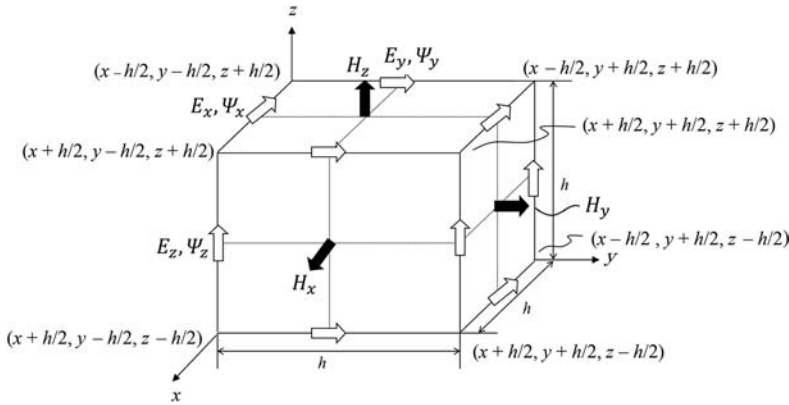


Figure 12.3 Positions of the three components of the magnetic field $\mathbf{H}$, electric field $\mathbf{E}$, and Ψ on the unit cell of the 3D FDTD mesh; white arrows are for $\mathbf{E}$, and black arrows are for $\mathbf{H}$. The components are computed on a staggered grid.

d_q , $q = x, y, z$ are defined using the central difference formula, such as $d_x f_{x,y,z} = f_{x+1/2,y,z} - f_{x-1/2,y,z}$, etc., as explained in previous chapters. Using these substitutions, we find the $\mathbf{H}$ and $\mathbf{E}$ update equations as follows:

H update

$$H_x|_{x+h/2,y,z}^{\tau+1/2} = H_x|_{x+h/2,y,z}^{\tau-1/2} - \frac{\Delta t}{\mu h} \left(d_y E_z|_{x+h/2,y,z}^{\tau} - d_z E_y|_{x+h/2,y,z}^{\tau} \right), \quad (12.26a)$$

$$H_y|_{x,y+h/2,z}^{\tau+1/2} = H_y|_{x,y+h/2,z}^{\tau-1/2} - \frac{\Delta t}{\mu h} \left(d_z E_x|_{x,y+h/2,z}^{\tau} - d_x E_z|_{x,y+h/2,z}^{\tau} \right), \quad (12.26b)$$

$$H_z|_{x,y,z+h/2}^{\tau+1/2} = H_z|_{x,y,z+h/2}^{\tau-1/2} - \frac{\Delta t}{\mu h} \left(d_x E_y|_{x,y,z+h/2}^{\tau} - d_y E_x|_{x,y,z+h/2}^{\tau} \right). \quad (12.26c)$$

E update

$$E_x|_{x,y+h/2,z+h/2}^{\tau+1} = E_x|_{x,y+h/2,z+h/2}^{\tau} + \frac{\Delta t}{\epsilon_0 h} \left(d_y H_z|_{x,y+h/2,z+h/2}^{\tau+1/2} - d_z H_y|_{x,y+h/2,z+h/2}^{\tau+1/2} \right) - \frac{1}{\epsilon_0} d_t^f \Psi_x|_{x,y+h/2,z+h/2}^{\tau}, \quad (12.27a)$$

$$E_y|_{x+h/2,y,z+h/2}^{\tau+1} = E_y|_{x+h/2,y,z+h/2}^{\tau} + \frac{\Delta t}{\epsilon_0 h} \left(d_z H_x|_{x+h/2,y,z+h/2}^{\tau+1/2} - d_x H_z|_{x+h/2,y,z+h/2}^{\tau+1/2} \right) - \frac{1}{\epsilon_0} d_t^f \Psi_y|_{x+h/2,y,z+h/2}^{\tau}, \quad (12.27b)$$

$$E_z \Big|_{x+h/2, y+h/2, z}^{\tau+1} = E_z \Big|_{x+h/2, y+h/2, z}^{\tau} + \frac{\Delta t}{\epsilon_0 h} \left(d_x H_y \Big|_{x+h/2, y+h/2, z}^{\tau+1/2} - d_y H_x \Big|_{x+h/2, y+h/2, z}^{\tau+1/2} \right) - \frac{1}{\epsilon_0} d_t^f \Psi_z \Big|_{x+h/2, y+h/2, z}^{\tau}. \quad (12.27c)$$

Calculating c_1 and c_2 from the complex dielectric constant

For the $\Delta\Psi$ update, we need the values of c_1 and c_2 . In MRC-FDTD, the values of c_1 and c_2 change with the incident frequency. Let the complex dielectric constant at angular frequency ω be

$$\tilde{\epsilon} = \tilde{\epsilon}_r + i\tilde{\epsilon}_i, \quad (12.28)$$

where $\tilde{\epsilon}$ is experimentally determined and tabulated in various materials handbooks. Separating the real and imaginary parts of Eq. (12.2), and comparing with Eq. (12.28), we find that

$$\tilde{\epsilon}_r(\omega) = 1 - \frac{\omega_p^2}{v_c^2 + \omega^2}, \quad (12.29a)$$

$$\tilde{\epsilon}_i(\omega) = \frac{\omega_p^2 \nu_c}{\omega(\omega^2 + v_c^2)}. \quad (12.29b)$$

Solving Eq. (12.29) for ν_c and ω_p , and inserting the results into definition Eq. (12.17), we find that

$$c_2 = \exp\left(\frac{-\tilde{\epsilon}_i \omega \Delta t}{1 - \tilde{\epsilon}_r}\right), \quad (12.30a)$$

$$c_1 = \frac{\omega \Delta t}{\tilde{\epsilon}_i} \left[(1 - \tilde{\epsilon}_r)^2 + \tilde{\epsilon}_i^2 \right] (1 - c_2). \quad (12.30b)$$

The value of $\tilde{\epsilon}_i$ in Eq. (12.30) is positive. This form is appropriate for the first-order Drude model, given by Eq. (12.2).

From Eq. (12.19), we see that $\lim_{\tau \rightarrow \infty} \chi^\tau = \infty$ if $c_2 \geq 1$; thus, one (but not the only one) condition for algorithm stability is

$$c_2 < 1. \quad (12.31)$$

This condition always holds as long as $\tilde{\epsilon}_i > 0$, $\tilde{\epsilon}_r < 0$, and $\Delta t > 0$ from Eq. (12.30a).

12.3 MRC-FDTD for the Wave Equation in the TE Mode

In Chapter 10, we showed that Maxwell's equations in the TE mode ($E_x = E_y = H_z = 0$) for constant μ are equivalent to the wave equation even across material boundaries when $\tilde{\epsilon}$ is invariant along the z axis. Since FDTD for the wave equation is much easier (only E_z needs to be computed), we now proceed to develop MRC-FDTD for the wave equation.

Adding a conduction current and differentiating by time, Eq. (12.6b) becomes

$$\partial_t(\nabla \times \mathbf{H}) = \partial_t^2 \mathbf{D} + \sigma \partial_t \mathbf{E}, \quad (12.32)$$

where σ is the conductivity ($\mathbf{x}$ and t dependence are omitted for brevity). Taking the curl of both sides of Eq. (12.6a),

$$\begin{aligned} \mu \partial_t(\nabla \times \mathbf{H}) &= -\nabla \times (\nabla \times \mathbf{E}), \\ &= -\nabla^2 \mathbf{E}. \end{aligned} \quad (12.33)$$

Substituting for $\partial_t(\nabla \times \mathbf{H})$ from Eq. (12.32) into Eq. (12.33), we obtain

$$\mu(\partial_t^2 \mathbf{D} + \sigma \partial_t \mathbf{E}) = \nabla^2 \mathbf{E} + \nabla \times (\nabla \cdot \mathbf{E}). \quad (12.34)$$

In Eq. (12.34), we assume that $\nabla \cdot \mathbf{E} = 0$, which is true for highly conducting metals since they don't retain free charge.¹⁸ Replacing the derivatives with the finite difference approximations $\partial_t^2 \cong d_t^2/\Delta t^2$, $\nabla^2 \cong \mathbf{d}^2/h^2$, and $\partial_t f(t) \cong [f(t + \Delta t) - f(t - \Delta t)]/2\Delta t$ (d_t^2 and $\mathbf{d}^2$ are defined in Chapter 1), we obtain the difference equation model:

$$d_t^2 \mathbf{D}(t) + \frac{\sigma \Delta t}{2} [\mathbf{E}(t + \Delta t) - \mathbf{E}(t - \Delta t)] = \frac{\Delta t^2}{\mu h^2} \mathbf{d}^2 \mathbf{E}(t). \quad (12.35)$$

Discretizing time by $t = \tau \Delta t$ ($\tau = 0, 1, 2, \dots$), Eq. (12.35) becomes

$$\frac{\Delta t^2}{h^2 \mu} \mathbf{d}^2 \mathbf{E}^\tau = d_\tau^2 \mathbf{D}^\tau + \frac{\sigma \Delta t}{2} (\mathbf{E}^{\tau+1} - \mathbf{E}^{\tau-1}), \quad (12.36)$$

where $d_\tau^2 \mathbf{D}^\tau = \mathbf{D}^{\tau+1} + \mathbf{D}^{\tau-1} - 2\mathbf{D}^\tau$. From Eq. (12.11),

$$d_\tau^2 \mathbf{D}^\tau = \epsilon_0 d_\tau^2 \mathbf{E}^\tau + d_\tau^2 \Psi^\tau. \quad (12.37)$$

Inserting Eq. (12.37) into Eq. (12.36), the difference equation model becomes

$$\epsilon_0 d_\tau^2 \mathbf{E}^\tau + \frac{\sigma \Delta t}{2} (\mathbf{E}^{\tau+1} - \mathbf{E}^{\tau-1}) = \frac{\Delta t^2}{h^2 \mu} \mathbf{d}^2 \mathbf{E}^\tau - d_\tau^2 \Psi^\tau. \quad (12.38)$$

Expanding $d_\tau^2 \mathbf{E}^\tau$ and solving for $\mathbf{E}^{\tau+1}$, we obtain a recursive convolution algorithm to solve the wave equation:

$$\mathbf{E}^{\tau+1} = -\left(\frac{1 - \alpha \Delta t}{1 + \alpha \Delta t}\right) \mathbf{E}^{\tau-1} + \frac{1}{1 + \alpha \Delta t} \left(2\mathbf{E}^\tau + \frac{\nu^2 \Delta t^2}{h^2} \mathbf{d}^2 \mathbf{E}^\tau - \frac{1}{\epsilon_0} d_\tau^2 \Psi^\tau\right), \quad (12.39)$$

where $\alpha = \sigma/2\epsilon_0$, and $\nu^2 = 1/\mu\epsilon_0$. From Eq. (12.24), applying a forward difference operator on both sides, we find that

$$d_\tau^2 \Psi^\tau = c_1(\mathbf{E}^\tau - \mathbf{E}^{\tau-1}) + c_2 d_\tau^2 \Psi^{\tau-1}, \quad (12.40)$$

and thus obtain the update

$$\Psi^{\tau+1} + \Psi^{\tau-1} - 2\Psi^\tau = c_1(\mathbf{E}^\tau - \mathbf{E}^{\tau-1}) + c_2(\Psi^\tau + \Psi^{\tau-2} - 2\Psi^{\tau-1}). \quad (12.41)$$

For $\mathbf{E} = \hat{\mathbf{z}} E_z$, $E_z = E_z(x, y, t)$, Eqs. (12.39) and (12.40) reduce to

$$\begin{aligned} E_z^{\tau+1} = & -\left(\frac{1 - \alpha \Delta t}{1 + \alpha \Delta t}\right) E_z^{\tau-1} \\ & + \frac{1}{1 + \alpha \Delta t} \left(2E_z^\tau + \frac{\nu^2 \Delta t^2}{h^2} \mathbf{d}^2 E_z^\tau - \frac{1}{\epsilon_0} d_\tau^2 \Psi_z^\tau\right), \end{aligned} \quad (12.42a)$$

$$d_\tau^2 \Psi_z^{\tau+1} = c_1(E_z^{\tau+1} - E_z^\tau) + c_2 d_\tau^2 \Psi_z^\tau. \quad (12.42b)$$

12.4 Stability of MRC-FDTD

Let us define the (dimensionless) grid velocity to be $u = \nu \Delta t/h$. As we saw in Appendix 7.1, the value of u determines the stability of the FDTD algorithm. In 2D/3D S-FDTD (neglecting dispersion), the stability condition is $u \leq 1/\sqrt{d}$, where d is the number of dimensions. But when dispersion is included, this condition might not hold, at least for some shorter wavelengths.

Using $\Delta \Psi^\tau = \Psi^{\tau+1} - \Psi^\tau = d_\tau \Psi^{\tau+1/2}$, the update equations for $\mathbf{E}$ and Ψ in Eq. (12.25) can be recast into the form

$$\mathbf{E}^{\tau+1} = \mathbf{E}^{\tau} - \frac{1}{\varepsilon_0} d_{\tau} \Psi^{\tau+1/2} + \frac{\Delta t}{\varepsilon_0 h} \mathbf{d} \times \mathbf{H}^{\tau+1/2}, \quad (12.43a)$$

$$d_t \Psi^{\tau+3/2} = c_1 \mathbf{E}^{\tau+1} + c_2 d_t \Psi^{\tau+1/2} \quad (12.43b)$$

and combined with the $\mathbf{H}$ update [Eq. (12.25a)] into the compact form

$$\mathbf{F}^{\tau+1} = \mathbf{M}\mathbf{F}^{\tau} + \mathbf{N}\mathbf{F}^{\tau+1}, \quad (12.44)$$

$$\mathbf{F}^{\tau} = \begin{bmatrix} \mathbf{H}^{\tau-1/2} \\ \mathbf{E}^{\tau} \\ d_{\tau} \Psi^{\tau+1/2} \end{bmatrix}, \mathbf{M} = \begin{bmatrix} 1 & -\mathbf{p} & 0 \\ 0 & 1 & -1 \\ 0 & 0 & c_2 \end{bmatrix}, \mathbf{N} = \begin{bmatrix} 0 & 0 & 0 \\ \mathbf{q} & 0 & 0 \\ 0 & c_1 & 0 \end{bmatrix}, \quad (12.45)$$

where $\mathbf{p} = (\Delta t/\mu_0 h) \mathbf{d} \times$, and $\mathbf{q} = (\Delta t/\varepsilon_0 h) \mathbf{d} \times$. In Appendix 12.2, we assign numerical meanings to $\mathbf{p}$ and $\mathbf{q}$, but for now we regard them as abstract quantities.

Solving Eq. (12.44) for $\mathbf{F}^{\tau+1}$, we find that

$$\begin{aligned} \mathbf{F}^{\tau+1} &= (\mathbf{I} - \mathbf{N})^{-1} \mathbf{M} \mathbf{F}^{\tau}, \\ &= \mathbf{C} \mathbf{F}^{\tau}, \end{aligned} \quad (12.46)$$

where $\mathbf{I}$ is the identity matrix, $(\mathbf{I} - \mathbf{N})^{-1}$ is the inverse of $(\mathbf{I} - \mathbf{N})$, and $\mathbf{C} = (\mathbf{I} - \mathbf{N})^{-1} \mathbf{M}$. We find that

$$(\mathbf{I} - \mathbf{N})^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ \mathbf{q} & 1 & 0 \\ c_1 \mathbf{q} & c_1 & 1 \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 1 & -\mathbf{p} & 0 \\ \mathbf{q} & 1 - \mathbf{p}\mathbf{q} & -1 \\ c_1 \mathbf{q} & c_1(1 - \mathbf{p}\mathbf{q}) & c_2 - c_1 \end{bmatrix}. \quad (12.47)$$

The solution of Eq. (12.46) is

$$\mathbf{F}^{\tau} = \mathbf{C}^{\tau} \mathbf{F}^0. \quad (12.48)$$

If the MRC-FDTD algorithm is to be numerically stable, then $\mathbf{F}^{\tau}$ must remain finite as $\tau \rightarrow \infty$.

In Appendix 12.2 we show that the condition for stability is

$$\frac{v\Delta t}{h} \leq \frac{1}{\sqrt{8}} \cong 0.354 \text{ in three dimensions,} \quad (12.49a)$$

$$\frac{v\Delta t}{h} \leq \frac{1}{2} \text{ in two dimensions.} \quad (12.49b)$$

12.5 S-FDTD for Materials Described by Normal Dispersion

For lossy dielectric materials described by permittivities $\tilde{\varepsilon} = \tilde{\varepsilon}_r + i\tilde{\varepsilon}_i$, where $\tilde{\varepsilon}_r > 0$ and $\tilde{\varepsilon}_i > \tilde{\varepsilon}_r$, S-FDTD for Maxwell's equations derive from the following equations:

$$\mathbf{H}^{\tau+1/2} = \mathbf{H}^{\tau-1/2} - \frac{1}{\mu} \frac{\Delta t}{h} \mathbf{d} \times \mathbf{E}^\tau, \quad (12.50a)$$

$$\mathbf{E}^{\tau+1} = \frac{(1-\alpha)}{(1+\alpha)} \mathbf{E}^\tau + \frac{1}{(1+\alpha)} \frac{\Delta t}{\epsilon_0 h} \mathbf{d} \times \mathbf{H}^{\tau+1/2}. \quad (12.50b)$$

For the wave equation, the S-FDTD for this category of materials is derived from

$$\mathbf{E}^{\tau+1} = -\left(\frac{1-\alpha\Delta t}{1+\alpha\Delta t}\right) \mathbf{E}^{\tau-1} + \frac{1}{1+\alpha\Delta t} \left(2\mathbf{E}^\tau + \frac{\nu^2 \Delta t^2}{h^2} \mathbf{d}^2 \mathbf{E}^\tau\right), \quad (12.51)$$

where $\alpha = \tilde{\epsilon}_i / (2\epsilon_0 \tilde{\epsilon}_r)$, and $\nu^2 = 1/\mu\epsilon_0$.

12.6 Numerical Evaluation of Extinction and Scattering Cross-Sections

We used the MRC-FDTD described in the previous sections to compute the wavelength spectra of the extinction and scattering cross-sections for pairs and linear arrays of silver, right-circular nanocylinders in two dimensions. The results are discussed in the next chapter. In this section, we describe the formulations employed to numerically compute the extinction and scattering cross-sections using the output of MRC-FDTD calculations.

The scattering cross-section is given by¹⁹

$$C_s = \frac{W_s}{I_i}, \quad (12.52)$$

where I_i is incident irradiance (incident light intensity per unit area),

$$W_s = \oint_A \mathbf{S}_s \cdot \hat{\mathbf{n}} dA, \quad (12.53)$$

and $\mathbf{S}_s$ is the Poynting vector for the scattered light at each point. In three dimensions, A is a closed surface containing the scatterer, and $\hat{\mathbf{n}}$ is the outward normal on each point of A ; in two dimensions, A becomes a closed path surrounding the scatterer. From these definitions it is clear that the cross-section has units of length-squared (e.g., nm²) in three dimensions and length (e.g., nm) in two dimensions.

The Poynting vector for the scattered light is defined by

$$\mathbf{S}_s = \frac{1}{2} \text{Re}(\mathbf{E}_s \times \mathbf{H}_s^*). \quad (12.54)$$

For time-harmonic fields, this definition is equivalent to

$$\mathbf{S}_s = \frac{1}{T} \int_0^T [\text{Re}(\mathbf{E}_s) \times \text{Re}(\mathbf{H}_s)] dt. \quad (12.55)$$

This equivalence is proved below.

The extinction cross-section is defined to be¹⁹

$$C_e = \frac{W_e}{I_i}, \quad (12.56)$$

where

$$W_e = -\oint_A \mathbf{S}_e \cdot \hat{\mathbf{n}} dA, \quad (12.57)$$

and $\mathbf{S}_e$ is the Poynting vector associated with extinction and is defined by

$$\mathbf{S}_e = \mathbf{S}_t - \mathbf{S}_i - \mathbf{S}_s, \quad (12.58)$$

where $\mathbf{S}_t$ is the Poynting vector of the total fields (incident + scattered) at each point, and $\mathbf{S}_i$ is the Poynting vector of the incident field. Analogously to Eqs. (12.54) and (12.55),

$$\mathbf{S}_t = \frac{1}{2} \text{Re}(\mathbf{E}_t \times \mathbf{H}_t^*) = \frac{1}{T} \int_0^T [\text{Re}(\mathbf{E}_t) \times \text{Re}(\mathbf{H}_t)] dt, \quad (12.59)$$

$$\mathbf{S}_i = \frac{1}{2} \text{Re}(\mathbf{E}_i \times \mathbf{H}_i^*) = \frac{1}{T} \int_0^T [\text{Re}(\mathbf{E}_i) \times \text{Re}(\mathbf{H}_i)] dt. \quad (12.60)$$

Note 12.2

The Poynting vector for time-harmonic fields is

$$\mathbf{S} = \frac{1}{2} \text{Re}(\mathbf{E} \times \mathbf{H}^*). \quad (12.61)$$

For time-harmonic fields, $\mathbf{E}$ and $\mathbf{H}^*$ are given by

$$\mathbf{E} = \mathbf{E}_0 \exp[i(\mathbf{k} \cdot \mathbf{x} - \omega t)], \quad (12.62)$$

$$\mathbf{H}^* = \mathbf{H}_0 \exp[-i(\mathbf{k} \cdot \mathbf{x} - \omega t)], \quad (12.63)$$

where $\mathbf{E}_0$ and $\mathbf{H}_0$ are real vector fields. Hence,

$$\mathbf{S} = \frac{1}{2} \text{Re}(\mathbf{E} \times \mathbf{H}^*) = \frac{1}{2} (\mathbf{E}_0 \times \mathbf{H}_0). \quad (12.64)$$

Computing the time average of $\text{Re}(\mathbf{E}) \times \text{Re}(\mathbf{H})$, we find that

$$\frac{1}{T} \int_0^T [\text{Re}(\mathbf{E}) \times \text{Re}(\mathbf{H})] dt = \frac{1}{T} \int_0^T (\mathbf{E}_0 \times \mathbf{H}_0) \cos^2(\mathbf{k} \cdot \mathbf{r} - \omega t) dt. \quad (12.65)$$

Defining $u = c - \omega t$, it follows that $-\omega dt = du$; hence, as $t \rightarrow 0$, $u \rightarrow c$, and as $t \rightarrow T$, $u \rightarrow c - \omega T$. Using $\cos 2u = \cos^2 u - \sin^2 u = \cos^2 u - (1 - \cos^2 u)$, which implies that $\cos^2 u = (1 + \cos 2u)/2$, Eq. (12.65) can now be transformed into

$$\begin{aligned} \frac{1}{T} \int_0^T [\text{Re}(\mathbf{E}) \times \text{Re}(\mathbf{H})] dt &= -\frac{1}{2\omega T} \int_c^{c-\omega T} (\mathbf{E}_0 \times \mathbf{H}_0) [1 + \cos(2u)] du \\ &= -\frac{1}{2\omega T} (\mathbf{E}_0 \times \mathbf{H}_0) (c - \omega T - c) \\ &= \frac{1}{2} (\mathbf{E}_0 \times \mathbf{H}_0). \end{aligned} \quad (12.66)$$

Computing Poynting vectors ($\mathbf{S}$)

Next, let us discuss the actual implementation of Eq. (12.66) to compute the Poynting vector using the electric and magnetic fields computed by FDTD:

$$\text{Re}(\mathbf{E}) \times \text{Re}(\mathbf{H}) = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \text{Re}(E_x) & \text{Re}(E_y) & \text{Re}(E_z) \\ \text{Re}(H_x) & \text{Re}(H_y) & \text{Re}(H_z) \end{vmatrix}. \quad (12.67)$$

Writing $\text{Re}(E_j) = E_j^r$ ($j = x, y, z$), we obtain

$$\begin{aligned} \text{Re}(\mathbf{E}) \times \text{Re}(\mathbf{H}) &= \hat{x} (E_y^r H_z^r - E_z^r H_y^r) + \hat{y} (E_z^r H_x^r - E_x^r H_z^r) \\ &\quad + \hat{z} (E_x^r H_y^r - E_y^r H_x^r) \\ &= \hat{x} S_x + \hat{y} S_y + \hat{z} S_z, \end{aligned} \quad (12.68)$$

$$\begin{aligned} S_x &= E_y^r H_z^r - E_z^r H_y^r, \\ S_y &= E_z^r H_x^r - E_x^r H_z^r, \\ S_z &= E_x^r H_y^r - E_y^r H_x^r. \end{aligned} \quad (12.69)$$

In 2D, for the TM mode, $H_x = H_y = E_z = 0$; hence,

$$S_x = E_y^r H_z^r, S_y = -E_x^r H_z^r, S_z = 0. \quad (12.70)$$

From Eqs. (12.64) and (12.66), we can write

$$\frac{1}{T} \int_0^T [\text{Re}(\mathbf{E}) \times \text{Re}(\mathbf{H})] dt = \frac{1}{T} \int_0^T (\hat{\mathbf{x}}S_x + \hat{\mathbf{y}}S_y + \hat{\mathbf{z}}S_z) dt. \quad (12.71)$$

In Eq. (12.71) S_x , S_y , and S_z are given by Eq. (12.69) in 3D, and by Eq. (12.70) in 2D.

To compute the intensities of E_x^2 and E_y^2 , we can use the same arguments given above and write the following relations:

$$\frac{1}{T} \int_0^T E_x^2 dt = \frac{1}{T} \int_0^T (E_x^r)^2 dt, \quad (12.72)$$

$$\frac{1}{T} \int_0^T E_y^2 dt = \frac{1}{T} \int_0^T (E_y^r)^2 dt. \quad (12.73)$$

FDTD programs output the electromagnetic field components at each time step. To compute field intensities and the Poynting vector from this data, numerical methods are needed. The time average of S_x , S_y , E_x^2 , and E_y^2 in the 2D TM mode are given by

$$\langle S_x \rangle = \sum_{t=0}^{nT} (E_y^r H_z^r), \quad (12.74)$$

$$\langle S_y \rangle = \sum_{t=0}^{nT} (-E_x^r H_z^r), \quad (12.75)$$

$$\langle E_x^2 \rangle = \sum_{t=0}^{nT} (E_x^r)^2, \quad (12.76)$$

$$\langle E_y^2 \rangle = \sum_{t=0}^{nT} (E_y^r)^2, \quad (12.77)$$

where n is an integer, T is the wave period, and angular brackets denote the time average of the corresponding quantities.

The above method for computing the time average of the Poynting vector is particularly effective when the spatial grid resolution is small (typically 0.5 nm or 1 nm up to a few nanometers).

Using Eqs. (12.62)–(12.64) and (12.6), it can be shown that the total intensity I equals the magnitude of the Poynting vector at each point of the spatial grid. $I = |\mathbf{E}|^2 = E_x^2 + E_y^2 + E_z^2$ is given by

$$I = \frac{1}{n} |\mathbf{S}| = \frac{1}{n} \sqrt{S_x^2 + S_y^2 + S_z^2}, \quad (12.78)$$

where n is the refractive index of the medium in which the observation is made.

Note that when the Poynting vector is computed using Eqs. (12.74) and (12.75), the direction of flux at each point and the effect of the refractive index of the medium are included. This information is incorporated in the electric field intensities alone. Furthermore, it should be noted that E_x , E_y , and H_z are not computed on exactly the same spatial grid point. For greater accuracy, while computing the components of the Poynting vector, interpolation of the field components might be needed.

Computing the cross-sections of scattering C_s and extinction C_e

The components of the various Poynting vectors are computed using FDTD. Using Eqs. (12.54) and (12.55), these components are computed by numerically evaluating the contour integral along a rectangular path surrounding the scatterer (particles). Especially for larger particles, the closed-path integral is needed to account for the relatively large amount of scattering.

The closed contour is shown in Fig. 12.4. By convention, the path integral is evaluated in the anticlockwise direction indicated by the arrows in Fig. 12.4. Otherwise, the result would be negative. In Fig. 12.4, $y_2 > y_1$ and $x_2 > x_1$.

We now evaluate $\mathbf{S}$ on the contour of Fig. 12.4 and obtain

$$\begin{aligned}
 W &= \oint_A \mathbf{S} \cdot \hat{\mathbf{n}} \, dA = \int_{y_1}^{y_2} \mathbf{S} \cdot \hat{\mathbf{x}} \, dy + \int_{x_1}^{x_2} \mathbf{S} \cdot \hat{\mathbf{y}} \, dx + \int_{y_1}^{y_2} \mathbf{S} \cdot (-\hat{\mathbf{x}}) \, dy + \int_{x_1}^{x_2} \mathbf{S} \cdot (-\hat{\mathbf{y}}) \, dx \\
 &= \int_{y_1}^{y_2} S_x|_{x_2} \, dy + \int_{x_1}^{x_2} S_y|_{y_2} \, dx - \int_{y_1}^{y_2} S_x|_{x_1} \, dy - \int_{x_1}^{x_2} S_y|_{y_1} \, dx.
 \end{aligned} \tag{12.79}$$

The trapezoidal rule for numerical integration is given by

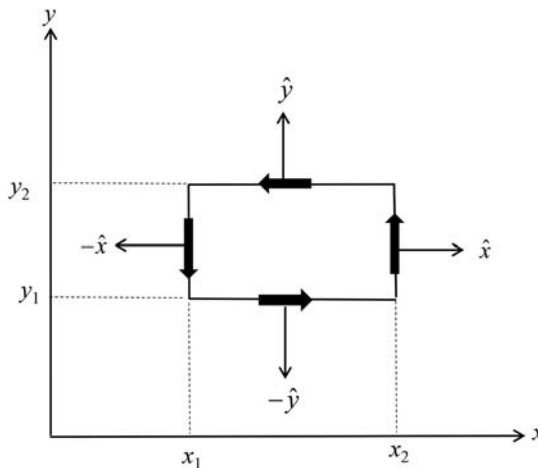


Figure 12.4 The reference frame and the contour for the closed integral.

$$\int_a^b f(x)dx = \frac{b-a}{N} \left\{ \sum_{i=1}^{N-1} f(x_i) + 0.5[f(x_0) + f(x_N)] \right\}, \quad (12.80)$$

where $b = a + N\Delta x$, and Δx is the sampling interval. The factor $(b-a)/N$ determines the sign of the integral.

Using the trapezoidal rule [Eq. (12.80)] to approximate the integrals in Eq. (12.79), we find that

$$\begin{aligned} W &= \oint_A \mathbf{S} \cdot \hat{\mathbf{n}} dA \\ &\cong \sum_{y=y_1+1}^{y_2-1} \langle E_y^r H_z^r |_{x_2} \rangle + 0.5 \left[\langle E_y^r H_z^r |_{x_2, y_1} \rangle + \langle E_y^r H_z^r |_{x_2, y_2} \rangle \right] \\ &\quad + \sum_{x=x_1+1}^{x_2-1} \langle -E_x^r H_z^r |_{y_2} \rangle + 0.5 \left[\langle -E_x^r H_z^r |_{x_1, y_2} \rangle + \langle -E_x^r H_z^r |_{x_2, y_2} \rangle \right] \\ &\quad - \sum_{y=y_1+1}^{y_2-1} \langle E_y^r H_z^r |_{x_1} \rangle - 0.5 \left[\langle E_y^r H_z^r |_{x_1, y_1} \rangle + \langle E_y^r H_z^r |_{x_1, y_2} \rangle \right] \\ &\quad - \sum_{x=x_1+1}^{x_2-1} \langle -E_x^r H_z^r |_{y_1} \rangle - 0.5 \left[\langle -E_x^r H_z^r |_{x_1, y_1} \rangle + \langle -E_x^r H_z^r |_{x_2, y_1} \rangle \right]. \end{aligned} \quad (12.81)$$

Note 12.3

It is important to remember that although the direction of the path changes along with the direction of the outward normal, the limits of integration do not change. Otherwise, the sign of the integral would remain the same, even if the path direction were reversed.

Outputs from the MRC-FDTD program (MC12.1_mrcFDTD) are as follows:

For scattered fields: $Intensx = \langle E_{s,y}^r H_{s,z}^r \rangle$, $Intensy = \langle -E_{s,z}^r H_{s,x}^r \rangle$,
 For total fields: $Intenx = \langle E_{t,y}^r H_{t,z}^r \rangle$, $Inteny = \langle -E_{t,x}^r H_{t,z}^r \rangle$,
 For incident fields: $Intenix = \langle E_{i,y}^r H_{i,z}^r \rangle$, $Inteniy = \langle -E_{i,x}^r H_{i,z}^r \rangle$.

Hence, using FDTD results,

$$\begin{aligned}
W_s = \oint_A \mathbf{S}_s \cdot \hat{\mathbf{n}} \, dA \cong & \sum_{y=y_1+1}^{y_2-1} \text{Intens}x|_{x_2} + 0.5(\text{Intens}x|_{x_2, y_1} + \text{Intens}x|_{x_2, y_2}) \\
& + \sum_{x=x_1+1}^{x_2-1} \text{Intens}y|_{y_2} + 0.5(\text{Intens}y|_{x_1, y_2} + \text{Intens}y|_{x_2, y_2}) \\
& - \sum_{y=y_1+1}^{y_2-1} \text{Intens}x|_{x_1} - 0.5(\text{Intens}x|_{x_1, y_1} + \text{Intens}x|_{x_1, y_2}) \\
& - \sum_{x=x_1+1}^{x_2-1} \text{Intens}y|_{y_1} - 0.5(\text{Intens}y|_{x_1, y_1} + \text{Intens}y|_{x_2, y_1}), \quad (12.82)
\end{aligned}$$

$$\begin{aligned}
\oint_A \mathbf{S}_t \cdot \hat{\mathbf{n}} \, dA \cong & \sum_{y=y_1+1}^{y_2-1} \text{Inten}x|_{x_2} + 0.5(\text{Inten}x|_{x_2, y_1} + \text{Inten}x|_{x_2, y_2}) \\
& - \sum_{y=y_1+1}^{y_2-1} \text{Inten}x|_{x_1} - 0.5(\text{Inten}x|_{x_1, y_1} + \text{Inten}x|_{x_1, y_2}) \\
& + \sum_{x=x_1+1}^{x_2-1} \text{Inten}y|_{y_2} + 0.5(\text{Inten}y|_{x_1, y_2} + \text{Inten}y|_{x_2, y_2}) \\
& - \sum_{y=y_1+1}^{y_2-1} \text{Inten}x|_{x_1} - 0.5(\text{Inten}x|_{x_1, y_1} + \text{Inten}x|_{x_1, y_2}), \quad (12.83)
\end{aligned}$$

$$\begin{aligned}
\oint_A \mathbf{S}_i \cdot \hat{\mathbf{n}} \, dA \cong & \sum_{y=y_1+1}^{y_2-1} \text{Inten}ix|_{x_2} + 0.5(\text{Inten}ix|_{x_2, y_1} + \text{Inten}ix|_{x_2, y_2}) \\
& + \sum_{x=x_1+1}^{x_2-1} \text{Inten}iy|_{y_2} + 0.5(\text{Inten}iy|_{x_1, y_2} + \text{Inten}iy|_{x_2, y_2}) \\
& - \sum_{y=y_1+1}^{y_2-1} \text{Inten}ix|_{x_1} - 0.5(\text{Inten}ix|_{x_1, y_1} + \text{Inten}ix|_{x_1, y_2}) \\
& - \sum_{x=x_1+1}^{x_2-1} \text{Inten}iy|_{y_1} - 0.5(\text{Inten}iy|_{x_1, y_1} + \text{Inten}iy|_{x_2, y_1}). \quad (12.84)
\end{aligned}$$

Thus,

$$\begin{aligned}
 W_e &= -\oint_A \mathbf{S}_e \cdot \hat{\mathbf{n}} dA \\
 &= -\oint_A \mathbf{S}_t \cdot \hat{\mathbf{n}} dA + \oint_A \mathbf{S}_i \cdot \hat{\mathbf{n}} dA + \oint_A \mathbf{S}_s \cdot \hat{\mathbf{n}} dA.
 \end{aligned} \quad (12.85)$$

Computing I_i

$$I_i = \frac{1}{h(y_2 - y_1 + 1)} \sum_{y=y_1}^{y_2} (Inteniy)|_{x_2}, \quad (12.86)$$

where h is the spatial discretization in nanometers.

Scattering and extinction efficiency

The scattering efficiency Q_s and the extinction efficiency Q_e are dimensionless quantities obtained by dividing the corresponding cross-section values by the physical cross-sectional areas of the particles projected onto a plane normal to the direction of propagation of the incident light. These quantities are given by

$$Q_s = \frac{C_s}{\sigma}, \quad (12.87a)$$

$$Q_e = \frac{C_e}{\sigma}. \quad (12.87b)$$

For a sphere of radius a , the cross-sectional area is $\sigma = \pi a^2$; for infinite cylinders, in a 2D calculation, $\sigma = 2a$.

12.7 Reflection/Transmission of Thin Metal Films: MRC-FDTD versus Analytical Calculation

The reflection and transmission properties of a thin film layer can be computed from a 2×2 matrix known as a characteristic matrix.¹⁸ The elements of this matrix are obtained by implementing the boundary conditions on the electric and magnetic fields at any interface between two consecutive layers. The boundary conditions require that the tangential components of the electric and magnetic vectors be continuous across the interfaces.

Figures 12.5–12.7 show the wavelength spectra of reflection and transmission for gold, silver, and aluminum thin films, respectively, on a substrate of refractive index 1.5 computed using both the MRC-FDTD and the analytical characteristic matrix method¹⁸ in two dimensions.

The characteristic matrix $\mathbf{m}$ for a single thin layer is given by

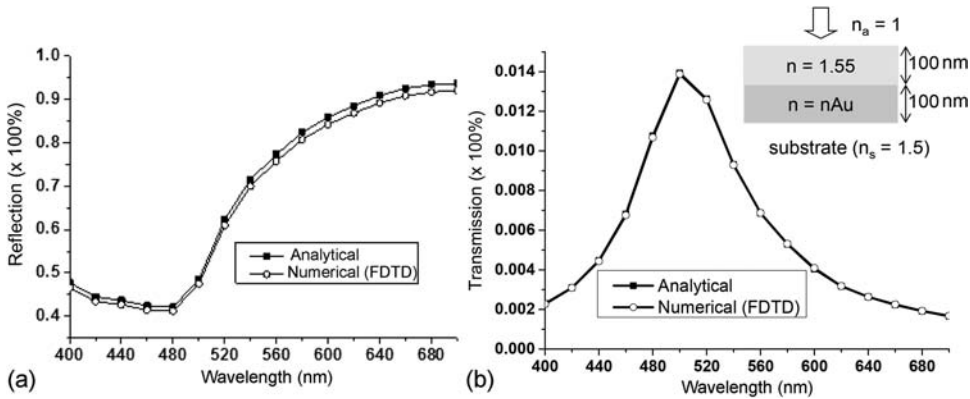


Figure 12.5 Wavelength spectra of (a) reflection and (b) transmission computed using the analytical characteristic matrix method and a numerical (FDTD) method. The inset shows a schematic of a two-layer thin film system comprising a dielectric layer of thickness 100 nm and refractive index 1.55, and a gold layer (n_{Au}) of thickness 100 nm.

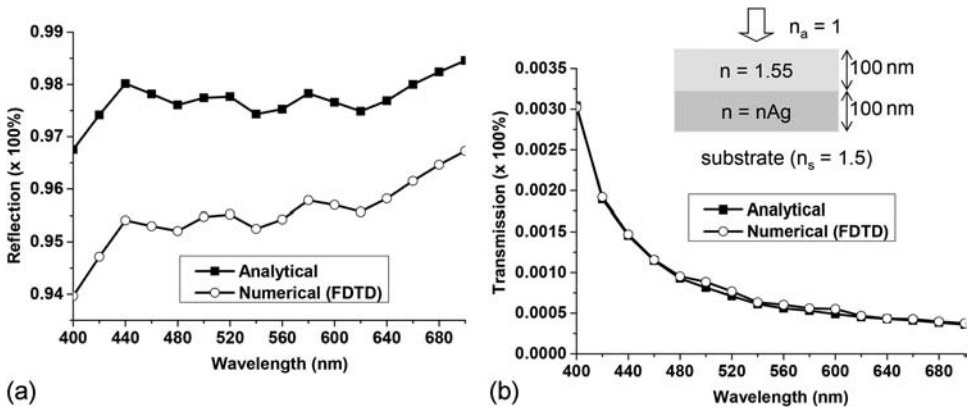


Figure 12.6 Wavelength spectra of (a) reflection and (b) transmission computed using the analytical characteristic matrix method and FDTD. The inset shows a schematic of a two-layer thin film system comprising a dielectric layer of thickness 100 nm and refractive index 1.55, and a silver layer (n_{Ag}) of thickness 100 nm.

$$\mathbf{m} = \begin{bmatrix} \cos\beta & -\frac{i}{\sqrt{\tilde{\epsilon}}} \sin\beta \\ -i\sqrt{\tilde{\epsilon}} \sin\beta & \cos\beta \end{bmatrix}. \quad (12.88)$$

For normal incidence, $\beta = (2\pi/\lambda)\sqrt{\tilde{\epsilon}}t$, where $\tilde{\epsilon}$ is the complex permittivity of the layer, t is the thickness (length along the propagation direction of light) of the layer, and λ is the wavelength of incident light. $\tilde{\epsilon}$ is obtained from a material handbook. For example, in Fig. 12.6, silver $\tilde{\epsilon}$ is obtained through cubic spline interpolation of the handbook permittivity (second set of data in

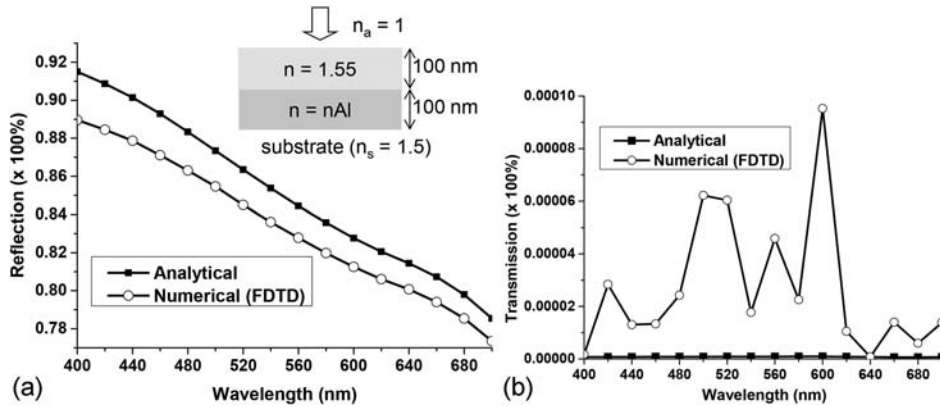


Figure 12.7 Wavelength spectra of (a) reflection and (b) transmission computed using the analytical characteristic matrix method and numerical (FDTD) method. The inset shows a schematic of a two-layer thin film system comprising a dielectric layer of thickness 100 nm and refractive index 1.55, and an aluminum layer (n_{Al}) of thickness 100 nm.

Fig. 12.2). Similar techniques are used for other metals, too. $\tilde{\epsilon}$ is the same for both TE and TM modes.

The characteristic matrix $\mathbf{M}$ for a system of two or more thin layers is given by

$$\begin{aligned} \mathbf{M} &= \prod_j \mathbf{m}_j \\ &= \begin{bmatrix} M_{1,1} & M_{1,2} \\ M_{2,1} & M_{2,2} \end{bmatrix}, \end{aligned} \quad (12.89)$$

where $\mathbf{m}_j$ is the characteristic matrix representing the j^{th} thin film of the multilayer and is computed from Eq. (12.88) using complex refractive indices and the thickness of the layer. In the TE mode, for normal incidence, the analytical reflection and transmission coefficients for the system are given, respectively, by

$$R = \left| \frac{n_a(M_{1,1} + n_s M_{1,2}) - (M_{2,1} + n_s M_{2,2})}{n_a(M_{1,1} + n_s M_{1,2}) + (M_{2,1} + n_s M_{2,2})} \right|^2, \quad (12.90)$$

$$T = \frac{n_s}{n_a} \left| \frac{2n_a}{n_a(M_{1,1} + n_s M_{1,2}) + (M_{2,1} + n_s M_{2,2})} \right|^2. \quad (12.91)$$

In Eqs. (12.90) and (12.91) n_a and n_s are the refractive indices of the incident medium and of the substrate, respectively. For normal incidence, R and T are same in TE and TM modes.

The comparisons in Figs. 12.5–12.7 between the analytical and FDTD computations show that the numerical simulation results can differ from

the analytical results by a maximum of 3% for reflection. The difference can be significant when values of transmission coefficients are too small [e.g., Fig. 12.7(b)].

12.8 Summary

In this chapter we discuss the implementation of a MRC-FDTD method and a new form of stability condition for the same. Compared to dispersionless FDTD, MRC-FDTD requires a shorter time step for numerical stability. We also discuss numerical methods to compute the extinction and scattering cross-sections using MRC-FDTD results.

Appendix 12.1 Eigenvalues and Eigenvectors of Matrices

Let the square matrix $\mathbf{A}$ have distinct eigenvalues λ_ℓ with the corresponding normalized eigenvectors $\boldsymbol{\lambda}_\ell$, where $\boldsymbol{\lambda}_\ell$ is a column matrix. By definition,

$$\mathbf{A}\boldsymbol{\lambda}_\ell = \lambda_\ell\boldsymbol{\lambda}_\ell. \quad (\text{A12.1.1})$$

Eigenvalues are called nontrivial if they do not equal zero, and nontrivial eigenvectors are nonzero vectors. We hereafter assume all eigenvalues and eigenvectors to be nontrivial.

The adjoint of $\mathbf{A}$ is defined to be $\mathbf{A}^\dagger = (\mathbf{A}^\top)^*$, where $\mathbf{A}^\top$ is the transpose of $\mathbf{A}$, and $*$ denotes the complex conjugate. If the elements of $\mathbf{A}$ are $(\mathbf{A})_{ij}$, then $(\mathbf{A}^\dagger)_{ij} = (\mathbf{A})_{ji}^*$. The adjoint of a column matrix $\mathbf{x}$ is the row matrix $\mathbf{x}^\dagger$, and $(\mathbf{x}^\dagger)_i = (\mathbf{x})_i^*$. We define the inner product of two vectors to be $\mathbf{x} \cdot \mathbf{y} = \mathbf{x}^\dagger \mathbf{y}$; hence, $\mathbf{y} \cdot \mathbf{x} = \mathbf{y}^\dagger \mathbf{x} = (\mathbf{x}^\dagger \mathbf{y})^\dagger = (\mathbf{x} \cdot \mathbf{y})^\dagger$. Thus, $\mathbf{x} \cdot \mathbf{x} \equiv |\mathbf{x}|^2$ is a real number and is the Euclidean magnitude of $\mathbf{x}$. When both $\mathbf{x}$ and $\mathbf{y}$ are real, then $\mathbf{x} \cdot \mathbf{y} = \mathbf{y} \cdot \mathbf{x}$.

Multiplying the left side of Eq. (A12.1.1) by $\boldsymbol{\lambda}_m^\dagger$ gives

$$\boldsymbol{\lambda}_m^\dagger \mathbf{A} \boldsymbol{\lambda}_\ell = \lambda_\ell \boldsymbol{\lambda}_m^\dagger \boldsymbol{\lambda}_\ell; \quad (\text{A12.1.2})$$

similarly,

$$\boldsymbol{\lambda}_\ell^\dagger \mathbf{A} \boldsymbol{\lambda}_m = \lambda_\ell \boldsymbol{\lambda}_\ell^\dagger \boldsymbol{\lambda}_m. \quad (\text{A12.1.3})$$

Taking the adjoint of Eq. (A12.1.3), we obtain

$$\boldsymbol{\lambda}_m^\dagger \mathbf{A}^\dagger \boldsymbol{\lambda}_\ell = \lambda_m^* \boldsymbol{\lambda}_\ell^\dagger \boldsymbol{\lambda}_m. \quad (\text{A12.1.4})$$

Subtracting Eq. (A12.1.4) from Eq. (A12.1.2), we obtain

$$\boldsymbol{\lambda}_m^\dagger (\mathbf{A} - \mathbf{A}^\dagger) \boldsymbol{\lambda}_\ell = \boldsymbol{\lambda}_m^\dagger \boldsymbol{\lambda}_\ell (\lambda_\ell - \lambda_m^*). \quad (\text{A12.1.5})$$

Hermitian matrix

$\mathbf{A}$ is called a Hermitian matrix if $\mathbf{A} = \mathbf{A}^\dagger$. If $\mathbf{A}$ is Hermitian, then Eq. (A12.1.5) gives

$$(\lambda_\ell - \lambda_m^*) \boldsymbol{\lambda}_m^\dagger \boldsymbol{\lambda}_\ell = 0. \quad (\text{A12.1.6})$$

Assuming the eigenvectors and eigenvalues to be nontrivial and distinct ($\ell \neq m \Rightarrow \lambda_\ell \neq \lambda_m$), it follows that $\ell = m \Rightarrow \lambda_\ell = \lambda_\ell^*$; hence, the eigenvalues of a Hermitian matrix are real. Since the eigenvalues are real, $\ell \neq m \Rightarrow \boldsymbol{\lambda}_m^\dagger \boldsymbol{\lambda}_\ell = 0$.

The eigenvalues of a Hermitian matrix are thus real, and their corresponding eigenvectors are orthogonal. Assuming the number of eigenvalues to equal the dimension of the matrix, their eigenvectors span the space of the column vectors. Thus, an arbitrary vector $\mathbf{x}$ can be expanded in the form

$$\mathbf{x} = \sum_{\ell} a_{\ell} \boldsymbol{\lambda}_{\ell}, \quad (\text{A12.1.7})$$

where $a_{\ell} = \boldsymbol{\lambda}_{\ell}^\dagger \mathbf{x}$. Then using Eq. (A12.1.1), we obtain an expression for $\mathbf{A}$ raised to the power τ :

$$\mathbf{A}^{\tau} \mathbf{x} = \sum_{\ell} a_{\ell} \lambda_{\ell}^{\tau} \boldsymbol{\lambda}_{\ell}, \quad (\text{A12.1.8})$$

where $\tau = 0, 1, 2, \dots$

Non-Hermitian matrix

If $\mathbf{A}$ is non-Hermitian, but if the eigenvectors are linearly independent (mutually nonparallel, although not orthogonal), then $\mathbf{x}$ can still be expanded in the form of Eq. (A12.1.7), and expression Eq. (A12.1.8) holds; however, now the expansion coefficients are $a_{\ell} \neq \boldsymbol{\lambda}_{\ell}^T \mathbf{x}$.

For example, $\boldsymbol{\lambda}_1 = [1 \ 0]^T$ and $\boldsymbol{\lambda}_2 = [\cos \theta \ \sin \theta]^T$ are non-orthogonal, normalized, and linearly independent eigenvectors of

$$\mathbf{A} = \begin{bmatrix} \lambda_1 & \frac{(\lambda_2 - \lambda_1)}{\tan \theta} \\ 0 & \lambda_2 \end{bmatrix}, \quad (\text{A12.1.9})$$

which is non-Hermitian ($\tan \theta \neq 0$). A unit vector orthogonal to λ_1 is

$$\begin{aligned} \boldsymbol{\mu} &= \frac{1}{\sin \theta} (\boldsymbol{\lambda}_2 - \boldsymbol{\lambda}_1 \cos \theta) \\ &= [0 \ 1]^{\dagger}. \end{aligned} \quad (\text{A12.1.10})$$

An arbitrary vector $\mathbf{x} = [x \ y]^T$ can thus be expanded as

$$\begin{aligned}\mathbf{x} &= x\boldsymbol{\lambda}_1 + y\boldsymbol{\mu} \\ &= \left(x - \frac{y}{\tan \theta}\right)\boldsymbol{\lambda}_1 + \frac{y}{\sin \theta}\boldsymbol{\lambda}_2.\end{aligned}\quad (\text{A12.1.11})$$

Then,

$$\mathbf{A}^\tau \mathbf{x} = \left(x - \frac{y}{\tan \theta}\right)\lambda_1^\tau \boldsymbol{\lambda}_1 + \frac{y}{\sin \theta}\lambda_2^\tau \boldsymbol{\lambda}_2. \quad (\text{A12.1.12})$$

It is also interesting to note that

$$\mathbf{A}^\tau = \begin{bmatrix} \lambda_1^\tau & \frac{(\lambda_2^\tau - \lambda_1^\tau)}{\tan \theta} \\ 0 & \lambda_2^\tau \end{bmatrix}. \quad (\text{A12.1.13})$$

Appendix 12.2 MRC-FDTD Stability Analysis

Let matrix $\mathbf{A}$ represent the action of some algorithm on vector $\mathbf{x}$. From Eq. (A12.1.8), the condition that $\mathbf{x}$ remain finite as the algorithm is iterated is

$$|\lambda_j| \leq 1, \quad j = 0, 1, 2, \quad (\text{A12.2.1})$$

where λ_j are the eigenvalues of $\mathbf{A}$, and the corresponding eigenvectors are assumed to be linearly independent.

Using the results of Appendix A12.1, we can now analyze the stability of the MRC-FDTD algorithm described in Section 12.4. The matrix

$$\mathbf{C} = \begin{bmatrix} 1 & -\mathbf{p} & 0 \\ \mathbf{q} & 1 - \mathbf{p}\mathbf{q} & -1 \\ c_1\mathbf{q} & c_1(1 - \mathbf{p}\mathbf{q}) & c_2 - c_1 \end{bmatrix} \quad (\text{A12.2.2})$$

describes the action of the MRC-FDTD algorithm on $\mathbf{F}^\tau = [\mathbf{H}^{\tau-1/2} \quad \mathbf{E}^\tau \quad d_\tau \Psi^{\tau+1/2}]^\top$. Defining $u = c\Delta t/h$, where $c = 1/\sqrt{\mu_0\epsilon_0}$ is the speed of light, we seek a constraint on u such that $\lim_{\tau \rightarrow \infty} \mathbf{C}^\tau \mathbf{F}^0$ is finite.

To proceed we must assign values to the elements of $\mathbf{C}$. For the permittivity values $[\tilde{\epsilon}_r$ and $\tilde{\epsilon}_i$ in Eq. (12.30)] applicable to common metals in the visible domain, $c_2 \cong 1$ and c_1 must be very small. In the analysis presented here, we take $c_2 = 1$ and $c_1 \neq 0$.

We use the electromagnetic units introduced in Chapter 8, in which $\epsilon_0 = 1$ and $\mu_0 = 1/c^2$. For numerical convenience, in what follows we now choose units in which $c = 1$. From Section 12.4, we now have $\mathbf{p} = u\mathbf{d} \times$ and $\mathbf{q} = u\mathbf{d} \times$, where $\mathbf{p}$ and $\mathbf{p}\mathbf{q}$ act upon $\mathbf{E}$, and $\mathbf{q}$ acts upon $\mathbf{H}$ (see Section 12.4). Taking $\mathbf{E} = \hat{\mathbf{e}}\psi$, where $\psi = \exp[i(\omega t - \mathbf{k} \cdot \mathbf{x})]$, it follows that Maxwell's equation [Eq. (12.6a)] gives $\mathbf{H} = \hat{\mathbf{k}} \times \hat{\mathbf{e}}\psi$, where $\hat{\mathbf{e}}$ and $\hat{\mathbf{k}} = \mathbf{k}/k$ are unit vectors. Thus,

$$\mathbf{d} \times \mathbf{E} = -2i \sin(\mathbf{k}h/2) \times \hat{\mathbf{e}} \psi \quad (\text{A12.2.3})$$

where the j^{th} component ($j = x, y, z$) of vector $\sin(\mathbf{k}h/2)$ is $[\sin(\mathbf{k}h/2)]_j = \sin(k_j h/2)$.

Let us now take $\hat{\mathbf{k}} = \hat{\mathbf{x}}$ to be the propagation direction and $\hat{\mathbf{e}} = \hat{\mathbf{y}}$ to be the polarization of the electric field; then $\hat{\mathbf{k}} \times \hat{\mathbf{e}} = \hat{\mathbf{z}}$ is the polarization of the magnetic field, and

$$\mathbf{F}^\tau = [\hat{\mathbf{z}}\psi^{\tau-1/2} \quad \hat{\mathbf{y}}\psi^\tau \quad \hat{\mathbf{y}}d_\tau\Psi^{\tau+1/2}]^\text{T}. \quad (\text{A12.2.4})$$

Thus,

$$-\mathbf{d} \times \mathbf{E} = 2is_k \hat{\mathbf{z}}\psi, \quad (\text{A12.2.5a})$$

$$\mathbf{d} \times (\mathbf{d} \times \mathbf{E}) = 4s_k^2 \hat{\mathbf{y}}\psi, \quad (\text{A12.2.5b})$$

$$\mathbf{d} \times \mathbf{H} = 2is_k \hat{\mathbf{y}}\psi, \quad (\text{A12.2.5c})$$

where $s_k = \sin(kh/2)$. From Eqs. (A12.2.2) and (A12.2.4), we can write

$$\begin{aligned} \mathbf{C}\mathbf{F}^\tau &= \begin{bmatrix} 1 & -\mathbf{p} & 0 \\ \mathbf{q} & 1 - \mathbf{p}\mathbf{q} & -1 \\ c_1\mathbf{q} & c_1(1 - \mathbf{p}\mathbf{q}) & 1 - c_1 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{z}}\psi^{\tau-1/2} \\ \hat{\mathbf{y}}\psi^\tau \\ \hat{\mathbf{y}}d_\tau\Psi_y^{\tau+1/2} \end{bmatrix} \\ &= \begin{bmatrix} (\psi^{\tau-1/2} + 2ius_k\psi^\tau)\hat{\mathbf{z}} \\ \left\{ 2ius_k\psi^{\tau-1/2} + (1 - 4u^2s_k^2)\psi^\tau - d_\tau\Psi_y^{\tau+1/2} \right\}\hat{\mathbf{y}} \\ \left\{ c_1us_k\psi^{\tau-1/2} + c_1(1 - 4u^2s_k^2)\psi^\tau + (c_2 - c_1)d_\tau\Psi_y^{\tau+1/2} \right\}\hat{\mathbf{y}} \end{bmatrix}. \quad (\text{A12.2.6}) \end{aligned}$$

Thus, an effective form of $\mathbf{C}$ is

$$\mathbf{C} = \begin{bmatrix} 1 & 2ius_k\mathbf{f} & 0 \\ 2ius_k\mathbf{f} & 1 - 4u^2s_k^2 & -1 \\ c_12ius_k\mathbf{f} & c_1(1 - 4u^2s_k^2) & 1 - c_1 \end{bmatrix}, \quad (\text{A12.2.7})$$

where $\mathbf{f}$ is an operator such that $\mathbf{f}\hat{\mathbf{y}} = \hat{\mathbf{z}}$, $\mathbf{f}\hat{\mathbf{z}} = \hat{\mathbf{y}}$, and $\mathbf{f}\hat{\mathbf{x}} = \hat{\mathbf{x}}$ or $\mathbf{f}\hat{\mathbf{y}} = \hat{\mathbf{y}}$, implying that $|\mathbf{f}| = 1$. In the numerical analysis that follows, we set $|\mathbf{f}| = 1$.

To determine the value of u for which the algorithm is stable, we determine the eigenvalues of $\mathbf{C}$ by solving

$$\det \left\{ \mathbf{C} - \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix} \right\} = 0. \quad (\text{A12.2.8})$$

The solutions of Eq. (A12.2.8) are $\lambda_0 = 1$ and $\lambda_{\pm}$:

$$\lambda_{\pm} = \frac{1}{2} \left[2 - 4u^2 s_k^2 - c_1 \pm \sqrt{(4u^2 s_k^2 + c_1)(4u^2 s_k^2 + c_1 - 4)} \right]. \quad (\text{A12.2.9})$$

It can be verified that the eigenvectors are linearly independent so that Eq. (A12.1.8) applies; thus, the stability condition is given by Eq. (A12.2.1).

In order that $|\lambda_{\pm}| \leq 1$, we must require that $4u^2 s_k^2 + c_1 - 4 < 0 \Rightarrow$

$$u^2 < \frac{4 - c_1}{4 \max(s_k^2)}. \quad (\text{A12.2.10})$$

In the general case of $\mathbf{k} = \hat{\mathbf{x}} k_x + \hat{\mathbf{y}} k_y + \hat{\mathbf{z}} k_z$, where $k^2 = k_x^2 + k_y^2 + k_z^2$, $s_k \mathbf{f} \rightarrow \sin(\mathbf{k}h/2) \times$ and $s_k^2 \rightarrow \sin(\mathbf{k}h/2) \cdot \sin(\mathbf{k}h/2)$. This complicates the analysis because s_k becomes a vector, unlike the scalar case where $s_k s_k \neq s_k^2$. It can be shown that the stability condition becomes

$$u \leq \frac{1}{\sqrt{8}} \cong 0.354, \quad (\text{A12.2.11a})$$

$$u \leq \frac{1}{2} \quad (\text{A12.2.11b})$$

in two and three dimensions, respectively. These stability conditions have been numerically verified in numerous calculations.

Thus, when dispersion is included, the time step must be smaller compared to the dispersionless case.

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Chapter 13

Photonics Problems

In this chapter we employ the MRC-FDTD methodology developed in Chapter 12 to compute the interaction of light with metal nanostructures. Simulations of two different nanostructures are described in detail.

Topics:

- Simulation of metal nanoparticles
- Simulation of metal–insulator–metal (MIM) nanoresonators for color filtering

13.1 Simulation of Metal Nanoparticles

Arrays, clusters, or groups of metal nanoparticles can support localized surface plasmon resonance (LSPR) modes. The presence of these resonances and the ability to tune the wavelengths corresponding to the resonance peaks make metal nanoparticles particularly attractive for coloring. This application was well known to older civilizations, who used metal nanoparticles to color materials, as is evidenced in the production and use of stained-glass¹ or decorative items, such as the famous Lycurgus cup.²

LSPR occurs at an interface between a metal and a dielectric as a result of light–matter interaction, which is essentially a quantum mechanical phenomenon. However, as long as the structures considered are large enough to be described by a dielectric function (permittivity) that sums up the quantum mechanical properties of the material, surface plasmon resonances can be adequately described by classical electromagnetic theory.^{3,4} This is referred to as the weak-interaction regime in the literature. In the case of strong interactions that typically manifest when the dimensions of the structures are comparable to molecular dimensions, quantum theories are utilized.^{5,6}

In recent times, plasmonics is being harnessed to enhance the near fields and confine such fields in subwavelength regions.⁷ Presently, plasmon-enhanced sensing,⁸ fluorescence,^{9–11} LED emission,¹² photocatalysis,¹³ photoelectric effect in organic^{14,15} and inorganic solar cells, Raman scattering,¹⁶ Raman optical activity,⁶ graphene devices,¹⁷ and a host of other applications form very

active fields of research. One of the least expensive and easiest ways to fabricate a nanostructured plasmonic device is to employ arrays or clusters of nanoparticles.^{18–20}

Consequently, much effort was spent in characterizing arrays and clusters of nanoparticles both experimentally and through theory and numerical simulations.^{21–30} It is observed from both experiments and simulations that the positions and number of LSPR peaks of arrays or clusters of nanoparticles are decided by the structural parameters, such as the shape and size of each particle, the interparticle distances, and the polarization state of the incident light.

The LSPR properties of arrays or clusters of nanoparticles are studied by computing or measuring the extinction spectra. The extinction cross-section at each wavelength is an estimate of the fraction of incident light that is scattered and absorbed. The extinction spectra of a spherical particle can be computed analytically using Mie theory. No analytical closed-form solution exists for arbitrarily shaped particles or clusters of particles. For ellipsoidal particles within the quasi-static limit (small diameter compared to the wavelength of light), it is possible to compute optical cross-sections using approximate formulae.²⁷ In more general cases involving clusters or arbitrarily shaped particles, numerical methods, such as T-matrix,²⁸ discrete dipole approximation (DDA),²⁹ time-dependent density functional theory,³⁰ and FDTD³¹ are used.

In this section, we compute the extinction and scattering spectra of pairs of silver, infinite nanocylinders using the MRC-FDTD methodologies described in Chapter 12. These computations illustrate a way to extend the FDTD simulations to useful applications. The computation scheme presented here can be easily extended to particles of arbitrary shapes and clusters of particles in both two and three dimensions.^{32–35} The extinction/scattering spectra of a cluster of nanoparticles can reveal the average optical property of such clusters in composite media.

Figure 13.1 shows scattering and extinction spectra computed using Mie theory for two different infinite, right-circular nanocylinders with cross-sectional diameters $a = 40$ nm and 200 nm. This figure indicates that a larger diameter can shift the LSPR peak toward the longer wavelengths and can broaden the extinction/scattering spectra. As long as the particle considered is small compared to the wavelength, the scattering properties are more akin to those due to a dipole. As the particles become larger in size, scattering behavior due to quadrupole and higher-order poles becomes apparent.

Analytically (using Mie theory), C_e and C_s in the TE mode are given by³

$$C_s = \frac{\lambda}{\pi n_a} \left(b_0^2 + 2 \sum_{m=1}^N b_m^2 \right), \quad (13.1)$$

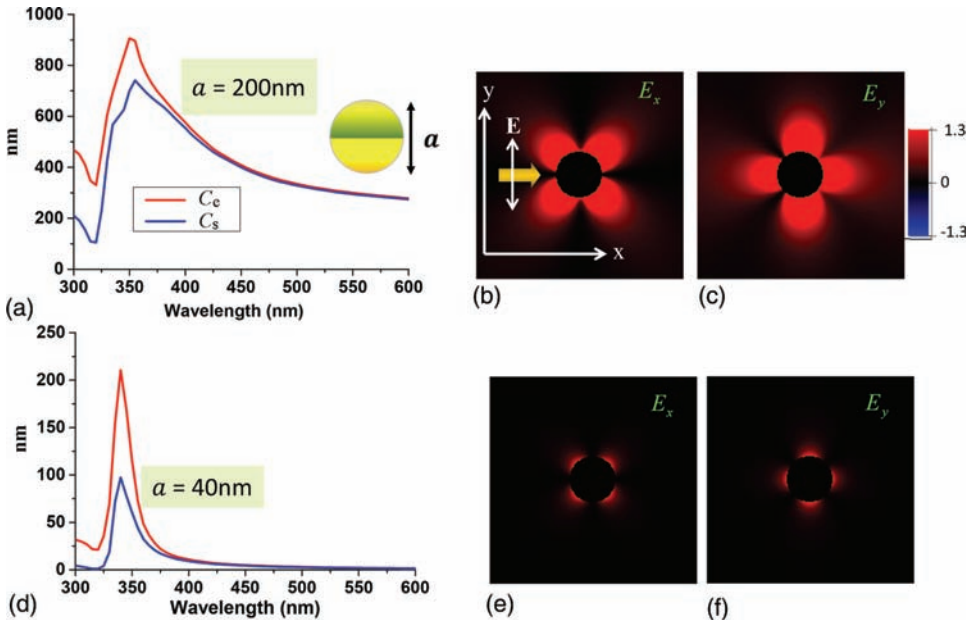


Figure 13.1 Mie theory used to compute the extinction cross-section C_e and scattering cross-section C_s of silver nanocylinders with cross-sectional diameter a of (a) 200 nm and (d) 40 nm in the TM mode; scattered intensity profile for (b) the x component and (c) the y component of the electric field at wavelength $\lambda = 340$ nm; (e) the x component and (f) the y component of the electric field at wavelength $\lambda = 580$ nm; (b), (c), (e), and (f) are computed for a nanocylinder with $a = 40$ nm.

$$C_e = \frac{\lambda}{\pi n_a} \operatorname{Re} \left(b_0 + 2 \sum_{m=1}^N b_m \right). \quad (13.2)$$

Similarly, C_e and C_s in the TM mode are given by³

$$C_s = \frac{\lambda}{\pi n_a} \left(\alpha_0^2 + 2 \sum_{m=1}^N \alpha_m^2 \right), \quad (13.3)$$

$$C_e = \frac{\lambda}{\pi n_a} \operatorname{Re} \left(\alpha_0 + 2 \sum_{m=1}^N \alpha_m \right), \quad (13.4)$$

where the coefficients b and α are functions of the diameter of the cross-section of the cylinder, the refractive index of the material of the cylinder, and the wavelength of incident light. The explicit forms of b and α are given by Eqs. (A10.1.26) and (A10.2.14) in Chapter 10. In Eqs. (13.1) to (13.4), n_a is the refractive index of the surrounding medium.

The analytical results shown in Figs. 13.1 and 13.3 are computed using Eqs. (13.3) and (13.4) [MC13.1_LSPRmie].

13.1.1 Simulations of pairs or arrays of nanocylinders

We can use MRC-FDTD to simulate pairs, arrays, or clusters of nanoparticles in both two and three dimensions. Some results are presented in this section.

The geometry in Fig. 13.2 is used to compute extinction cross-section spectra for pairs of nanocylinders in two dimensions. In all cases, the incident light is polarized in the TM mode or in the plane of the paper. The minimum resolution of the spatial grid is 0.5 nm, and the minimum resolution of the temporal grid is $\sim 0.33 \times 10^{-18}$ s. The incident beam is Gaussian with a beam waist of 250 nm and polarized along the y direction. The incident light is generated using a source current. We find that the position of the source current array significantly affects the nanocylinder characteristics. It is important to ensure that the current source is placed far enough from the surface of the metal nanocylinder that the current source does not significantly affect the scattered fields. It is also important to place the source at a safe distance from the left-side boundary of the simulation space. The source is placed 125 nm from the left-side boundary. The simulation space is terminated on all four sides with a slightly modified form of the nonstandard Mur absorbing boundary condition (ABC) described in Chapter 7.

In the computations presented here, a first-order version of the NS-Mur ABC [Eq. (7.107)] is used. The first-order formulation of the NS-Mur ABC is

$$\psi_{b,y}^{\tau+1} = \psi_{b,y}^{\tau} + \left(\psi_{i,y}^{\tau} - \psi_{i,y}^{\tau-1} \right) + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) \left[\left(\psi_{b,y}^{\tau} - \psi_{b,y}^{\tau-1} \right) - \left(\psi_{i,y}^{\tau+1} - \psi_{i,y}^{\tau} \right) \right], \quad (13.5a)$$

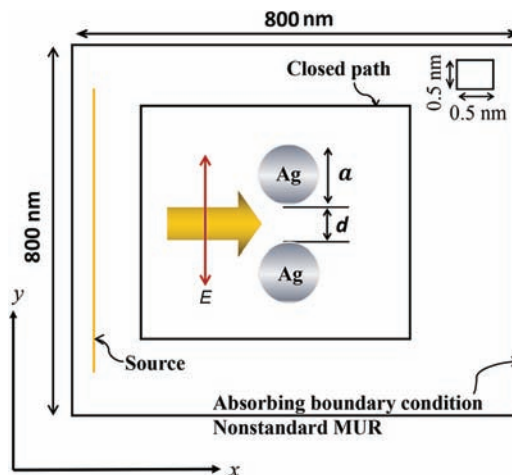


Figure 13.2 Computational geometry employed to simulate pairs of silver nanocylinders.

where $b = 0$ and $i = 1$ on the left, and $b = x_b$ and $i = x_b - 1$ on the right; and

$$\psi_{x,b}^{\tau+1} = \psi_{x,b}^{\tau} + \left(\psi_{x,i}^{\tau} - \psi_{x,i}^{\tau-1} \right) + \left(\frac{1 - \tilde{v}_1}{1 + \tilde{v}_1} \right) \left[\left(\psi_{x,b}^{\tau} + \psi_{x,b}^{\tau-1} \right) - \left(\psi_{x,i}^{\tau+1} - \psi_{x,i}^{\tau} \right) \right], \quad (13.5b)$$

where $b = 0$ and $i = 1$ on the bottom, and $b = y_b$ and $i = y_b - 1$ on the top. In Eq. (13.5), b denotes boundary, and i denotes interior. Space–time is discretized by taking $t = \tau \Delta t$ and $\mathbf{x} = (x, y)h$, where $\tau = 0, 1, 2, \dots$, $x = 0, 1, \dots, x_b$, $y = 0, 1, \dots, y_b$, and $x_b, y_b = b_x, b_y$.

In all simulations presented in this section, the complex refractive index of silver at a given wavelength is obtained using cubic interpolation of tabulated refractive index data for silver (data set 2 in Fig. 12.2). Because the tabulated data are specified at equal energy intervals, they were interpolated to the equal wavelength intervals used in the simulations. Computations were performed on the wavelength range 300–600 nm sampled at 10-nm intervals.

Figure 13.3(a) shows the extinction spectra computed for a silver nanocylinder in the TM mode using both Mie theory and MRC-FDTD. We computed the scattered electric field $\mathbf{E}_s = (E_x^s, E_y^s)$ and [in Figs. 13.3(b)–(e)] show the scattered intensity of each component, $|E_x^s|^2$ and $|E_y^s|^2$, for incident wavelengths $\lambda = 580$ and 340 nm. The cross-sectional diameter of all of the nanocylinders is $a = 40$ nm. The scattered fields depicted in Figs. 13.1 and 13.3 can be computed both numerically and analytically, and thus provide a check on the accuracy of the numerical calculations. Unfortunately, such checks are possible only for a single nanocylinder with a circular cross-section because

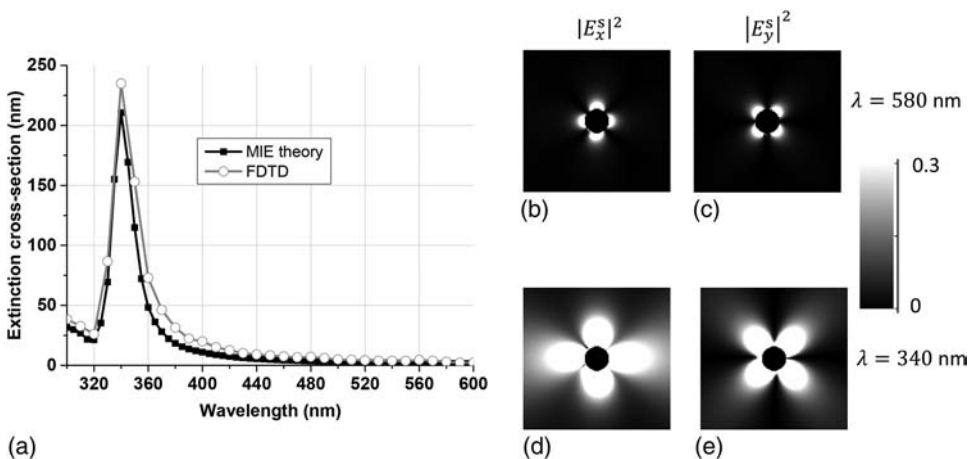


Figure 13.3 (a) Extinction spectra of a silver nanocylinder in the TM mode computed using Mie theory and MRC-FDTD; (b) and (d) show $|E_x^s|^2$ at $\lambda = 580$ and 340 nm, respectively; (c) and (e) show $|E_y^s|^2$ at $\lambda = 580$ and 340 nm, respectively. The intensity scale is shown on the right.

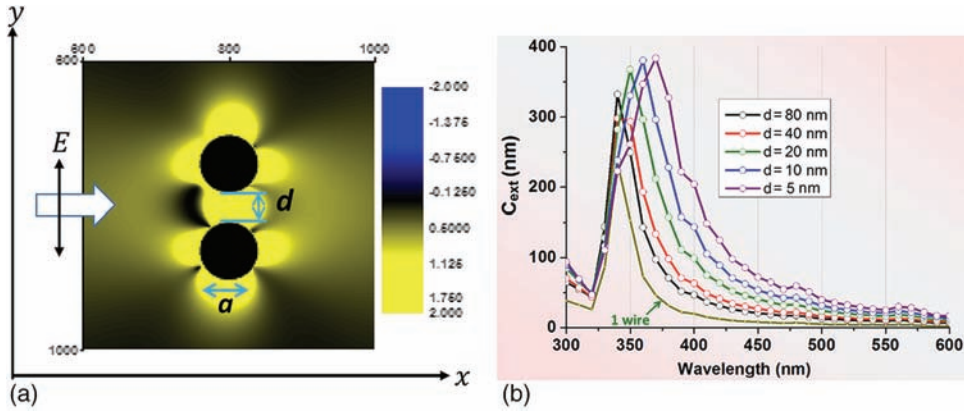


Figure 13.4 (a) $|E_y^s|^2$ around a nanocylinder pair for $d=20$ nm at the resonance peak; $\lambda = 350$ nm, and diameter $= a = 40$ nm for all the nanocylinders. (b) Extinction spectra for five pairs of nanocylinders in the TM mode; the gap d between the cylinders is varied in the following steps: 80 nm, 40 nm, 20 nm, 10 nm, and 5 nm. The incident field is an infinite plane wave propagating along the x axis, and the electric field of the incident light is polarized along the y axis. The propagation and polarization directions, the co-ordinate axes, and the parameters a and d are indicated in (a). The polarization direction of the incident light is parallel to the gap between the particles.

analytical solutions do not exist in a more general situation. The extinction cross-section C_e is computed numerically from FDTD simulations using the formulations described in Chapter 12.

Figure 13.4 shows the intensity distribution of the scattered field around a pair of nanocylinders and the extinction spectra computed for five pairs of right-circular, silver nanocylinders with five different interparticle distances d between the two cylinders forming the pair. d is varied in the following stages: 80 nm, 40 nm, 20 nm, 10 nm, and 5 nm. The cross-sectional diameter is $a = 40$ nm for all nanocylinders. In all cases, the polarization direction of the incident light is parallel to the gap between the two nanocylinders. The major peaks of the extinction spectra show a clear shift toward the longer wavelengths as the cylinders come closer to each other. At $d = 80$ nm, the peak is at the same wavelength as that due to a single nanocylinder, i.e., 340 nm. At $d = 5$ nm, the peak shifts to 370 nm, a 30-nm shift to the longer wavelength side. The red-shift is insignificant at relatively larger values of d and only becomes significant when d is fairly small. At smaller values of d , more than one peak can appear, indicating the presence of coupled modes.

Figure 13.5 shows the spatial distribution of $|E_x^s|^2$ and $|E_y^s|^2$ around the nanocylinders for $d = 80$ nm, 20 nm, and 2 nm. It is interesting to note that the electric field patterns change significantly as the cylinders come closer to each other. At $d = 2$ nm, the coupled cylinders behave more like a single, large cylinder; $a = 40$ nm in all cases.

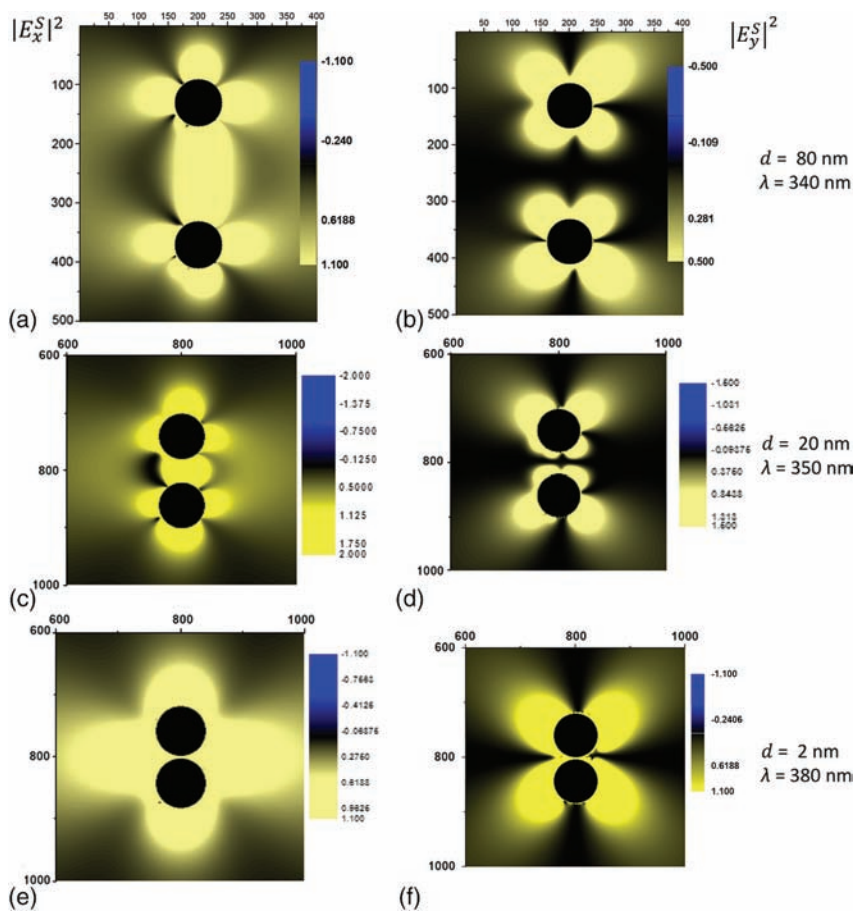


Figure 13.5 Computed spatial distribution of scattered intensity $|E_x^s|^2$ (left column) and $|E_y^s|^2$ (right column) around a nanowire pair; d =interparticle distance, and λ = incident wavelength.

Figure 13.6 shows the intensity distribution of the scattered field and the extinction spectra computed for five pairs of right-circular silver nanocylinders with five different interparticle distances d between the two cylinders forming the pair. d is varied in following stages: 20 nm, 10 nm, 5 nm, and 2 nm. The cross-sectional diameter of all of the nanocylinders is $a = 40$ nm. In all cases, the polarization direction of the incident light is normal to the gap between the two nanocylinders. For all values of d , the extinction spectra show only one major peak at $\lambda = 340$ nm, which comes out at the same position as the peak of a single nanocylinder with $a = 40$ nm at $\lambda = 340$ nm. Hence, when the polarization direction of the electric field is normal to the gap between the nanocylinders, it is impossible to shift the peak of the extinction spectra by bringing the cylinders closer to each other.

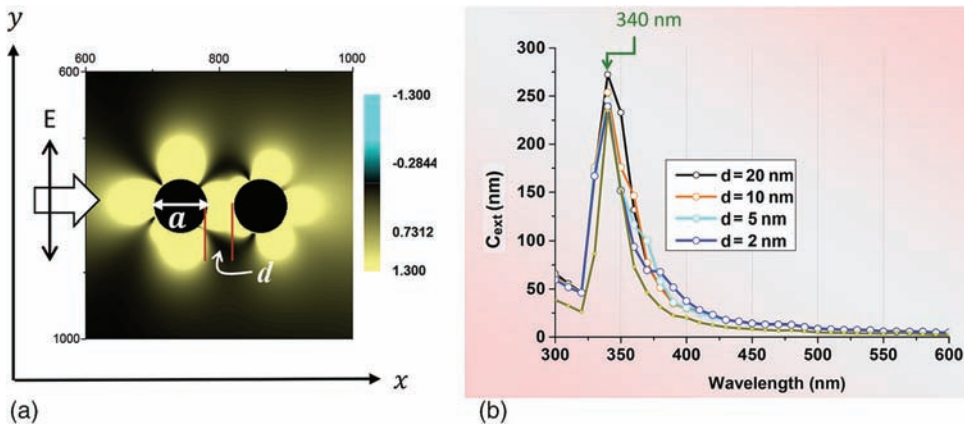


Figure 13.6 (a) Computed distribution of $|E_s|^2$ at $d = 20$ nm, $a = 40$ nm, and $\lambda = 340$ nm (resonance peak). (b) Extinction spectra for pairs of nanocylinders in the TM mode; $a = 40$ nm for all pairs, and $d = 20$ nm, 10 nm, 5 nm, and 2 nm. The incident field is along the x axis, and the electric field is polarized along the y axis. The propagation and polarization directions, the co-ordinate axes, and the parameters a and d are indicated in (a).

The aspect ratio of ellipsoids provides a useful degree of freedom with respect to tuning of LSPR peaks. Figure 13.7 shows the wavelength spectra of absorption cross-sections computed for small ellipsoids (length of semi-major axis is 40 nm and varying aspect ratio) using a quasi-static approximation for such particles.²⁷ Computing the absorption cross-section requires a calculation of associated Legendre polynomials of the first and second kind, which is performed in MC13.2_LSPRelipsoid. Figure 13.7 shows that increasing the aspect ratio shifts the absorption cross-section peak to longer wavelengths.

The MRC-FDTD computation model is also employed to simulate linear arrays of silver nanocylinders with elliptical and circular cross-sections.

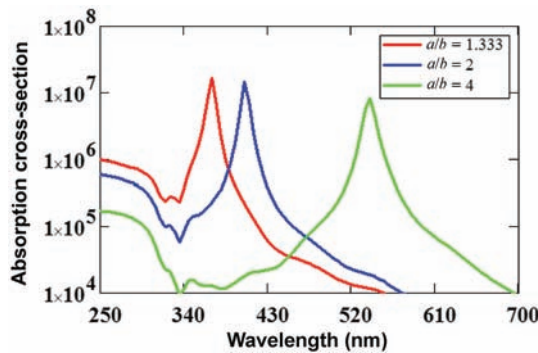


Figure 13.7 Wavelength spectra of absorption cross-sections for small ellipsoids; a is the semi-major axis length, and b is the length of the semi-minor axis. The peaks red-shift as the aspect ratio increases.

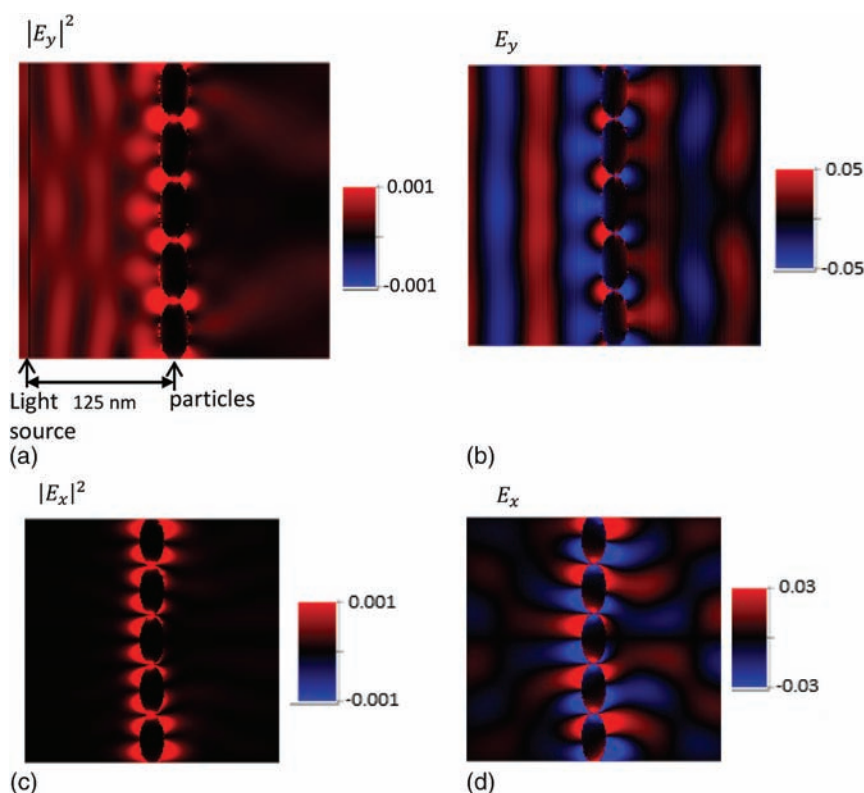


Figure 13.8 Linear array of five nanocylinders with elliptical cross-sections in the TM mode: (a) $|E_y|^2$, (b) E_y , (c) $|E_x|^2$, and (d) E_x . Incident light is y polarized, the wavelength of incident light is 420 nm, the lengths of the major and minor axes of the ellipses are 300 nm and 150 nm, respectively, and the gap between two contiguous nanocylinders is 5 nm.

Figures 13.8–13.10 present the results of the simulation of linear arrays of five, four, and three cylinders, respectively, with elliptical cross-sections in two dimensions. Such computations are especially useful in investigating field enhancement as a function of particle shape, size, interparticle distance, etc. The elliptical cross-sections considered in these calculations are large and are well beyond the quasi-static limit assumed in computing Fig. 13.7.

The simulation results presented in Figs. 13.8–13.10 can be compared with similar results obtained with linear arrays of five, four, and three nanocylinders with circular cross-sections. The simulation results for linear arrays of nanocylinders with large circular cross-sections (diameter = 300 nm) are presented in Figs. 13.11–13.13.

Figure 13.14 shows 3D simulations of the field enhancement due to a group of nanoparticles. Such simulations can show the effects (e.g., the reduced transmission) of cluster formation in composite material created by impregnating a homogeneous medium with nano-inclusions.³⁵ In Fig. 13.14,

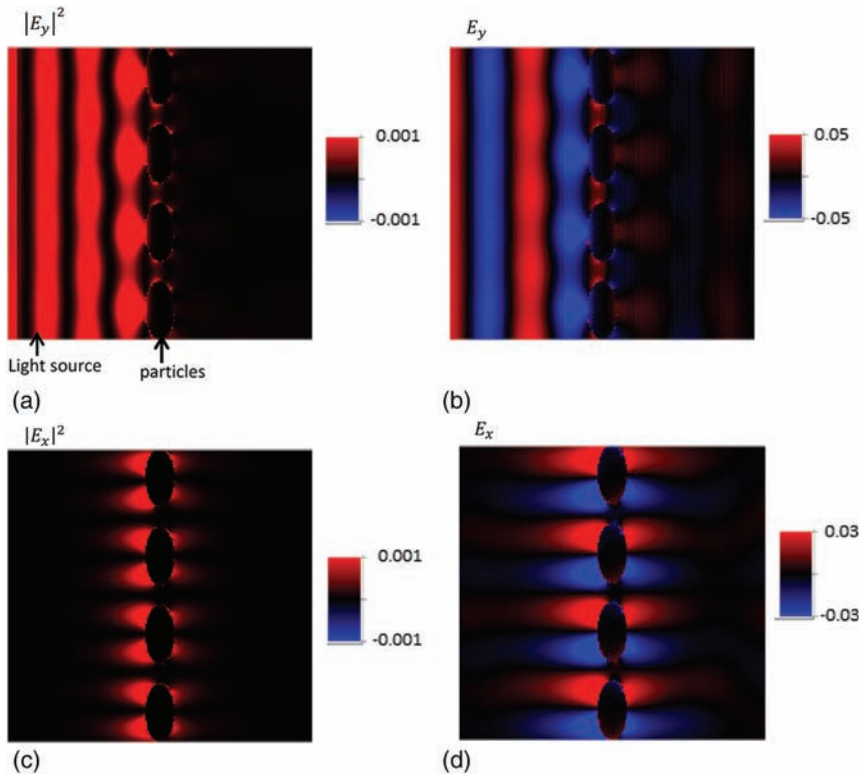


Figure 13.9 Linear array of four nanocylinders with elliptical cross-sections in the TM mode: (a) $|E_y|^2$, (b) E_y , (c) $|E_x|^2$, and (d) E_x . Incident light is y polarized, the wavelength of incident light is 420 nm, the lengths of the major and minor axes of the ellipses are 300 nm and 150 nm, respectively, and the gap between two contiguous nanocylinders is 100 nm.

the nanospherical silver inclusions are embedded in a homogeneous medium of refractive index 1.5.

13.2 Simulation of Metal–Insulator–Metal Nanoresonators for Color Filtering

Liquid crystal display (LCD) devices are ubiquitous in the form of computer, television, and mobile phone monitors. An essential component of an LCD device is the color filter, which determines the color saturation and quality of the image rendered by the LCD. Conventional color filters based on dye and pigment technology show broad transmission bandwidths and relatively low transmission.

In order to increase transmission over a narrower bandwidth, various color filter designs involving diffractive micro- and nano-grating structures are proposed in the literature. Guided-mode waveguide resonator structures are proposed as narrowband filters and polarizers.^{36,37} These structures exploit the cavity resonance modes for color filtering. Color filters have been

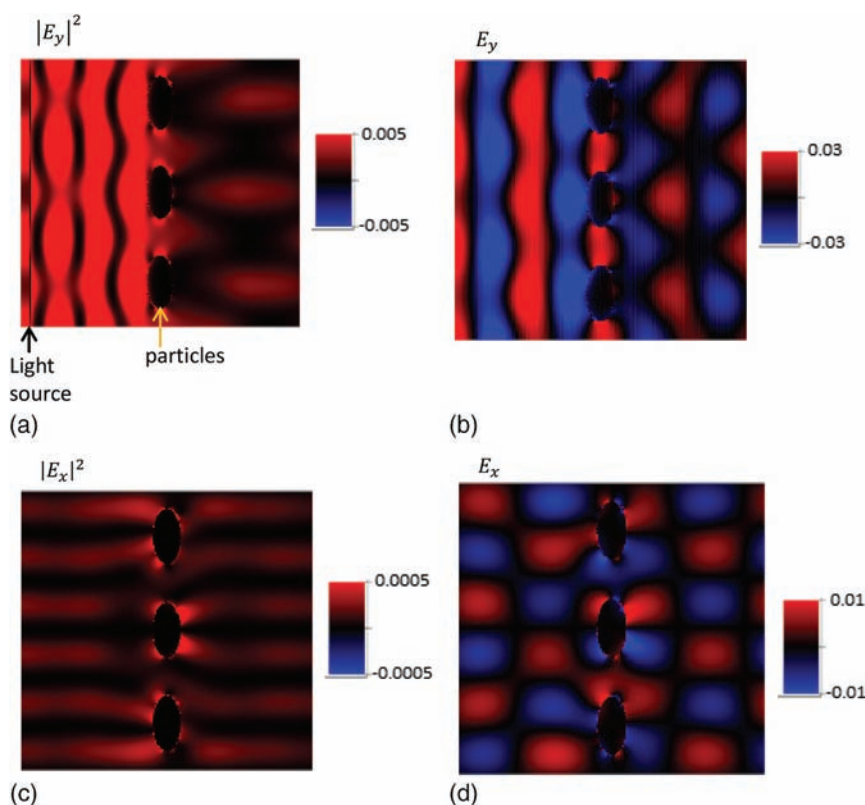


Figure 13.10 Linear array of three nanocylinders with elliptical cross-sections in the TM mode: (a) $|E_y|^2$, (b) E_y , (c) $|E_x|^2$, and (d) E_x . Incident light is y polarized, the wavelength of incident light is 420 nm, the lengths of the major and minor axes of the ellipses are 300 nm and 150 nm, respectively, and the gap between two contiguous nanocylinders is 200 nm.

implemented using both 2D and 1D subwavelength grating structures in both metallic films and silicon.^{38,39} Active color filtering was demonstrated using plasmonic metal nano-antennas.⁴⁰

Metal–insulator–metal (MIM)-layered structures have been proposed for color tuning the output from organic light-emitting diodes (OLEDs).⁴¹ Tunable color filters were designed using MIM structures.⁴² A MIM-based composite nanoresonator structure is proposed as a polarizing color filter.⁴³ The filtering behavior of such MIM-based devices is derived from surface plasmon resonances.

The structural design suggested in Ref. 43 employs high-refractive-index inorganic semiconducting material in the insulator layer. Also, the transmission bandwidths of these structures are relatively broad, limiting the purity of color that might be attained. Such material might be costly and might also involve optical loss. Figure 13.15 shows the composite nanoresonator structure proposed in Ref. 43 and the transmission spectra obtained in TE and TM

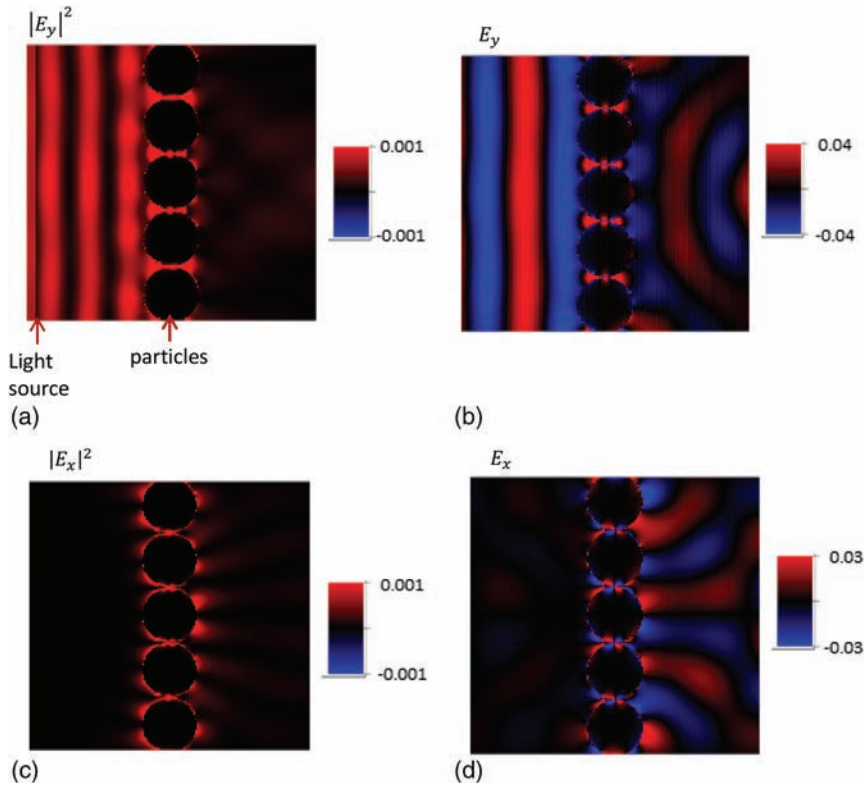


Figure 13.11 Linear array of five nanocylinders with circular cross-sections (diameter = 300 nm) in the TM mode: (a) $|E_y|^2$, (b) E_y , (c) $|E_x|^2$, and (d) E_x . Incident light is y polarized, the wavelength of incident light is 420 nm, and the gap between two contiguous nanocylinders is 5 nm.

modes with a high and a low refractive index value for the insulator layer. The insulator region is simulated as a dielectric material. The simulation results, particularly the transmission spectra in the TM mode, show that this structure can only be successful with an insulator layer of high refractive index.

We simulated slightly modified structures of MIM nanoresonators using relatively low-refractive-index polymeric materials in the insulator layer.^{44,45} From considerations of less-expensive material, a polymeric material is more desirable compared to a semiconducting inorganic material. However, high-refractive-index polymeric materials are rather unusual. Our simulations show that by modifying the structure in Fig. 13.15, it might be possible to obtain a filtering behavior with a MIM device implemented with a low-refractive-index material in the insulator layer. The simulations also show the effect of various design parameters on the transmission and reflection properties of these structures. The simulation results can be useful in designing MIM-based color-filtering structures.

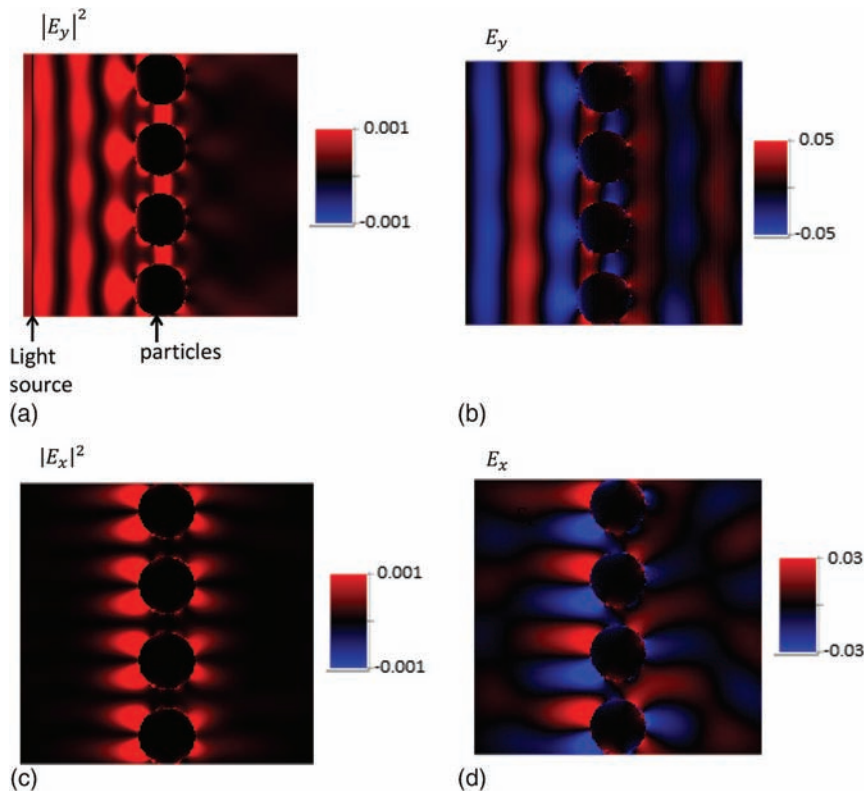


Figure 13.12 Linear array of four nanocylinders with circular cross-sections (diameter = 300 nm) in the TM mode: (a) $|E_y|^2$, (b) E_y , (c) $|E_x|^2$, and (d) E_x . Incident light is y polarized, the wavelength of incident light is 420 nm, and the gap between two contiguous nanocylinders is 100 nm.

13.2.1 Proposed structure

Figure 13.16 shows a schematic diagram of a slightly modified version of the structures shown in Fig. 13.15. The proposed structure can be seen as a 1D periodic layout of composite grating lines, where each grating line is composed of three layers with one insulator layer sandwiched between two thin metal layers. The openings between two contiguous composite grating lines are filled with the same insulator material. In simulations, the dispersive refractive index of aluminum is used in the metal layers.

13.2.2 Simulation results

The simulations are performed in two dimensions, assuming the structure to be infinitely periodic in one direction, finite along a normal direction, and invariant along a third direction perpendicular to the plane of the paper. In all simulations, the structure of Fig. 13.16 is assumed to sit on a substrate of refractive index 1.5.

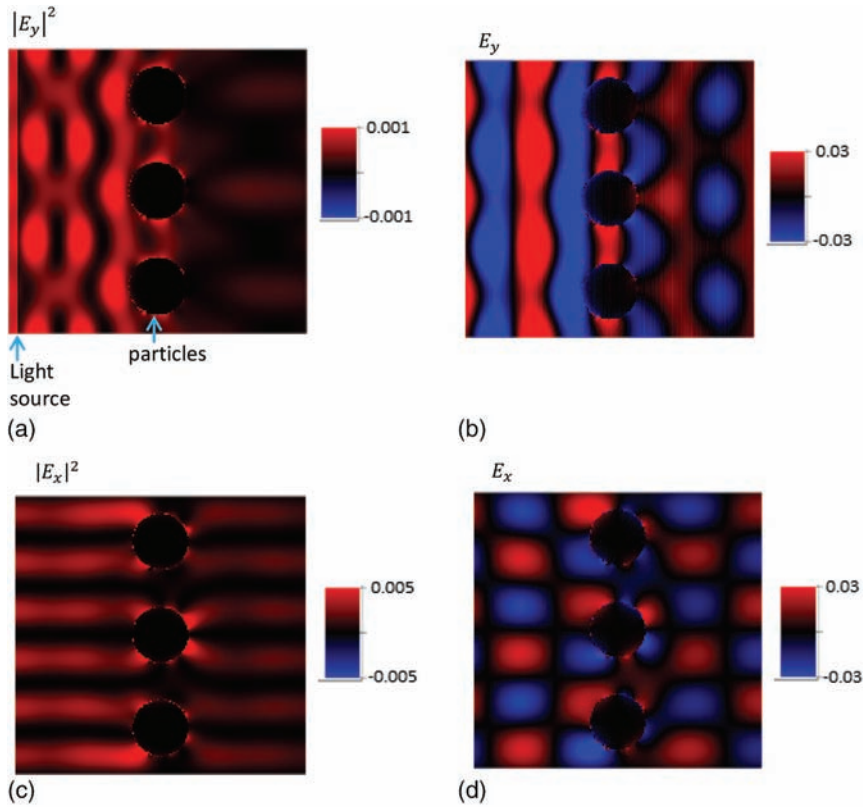


Figure 13.13 Linear array of three nanocylinders with circular cross-sections (diameter = 300 nm) in the TM mode: (a) $|E_y|^2$, (b) E_y , (c) $|E_x|^2$, and (d) E_x . Incident light is y polarized, the wavelength of incident light is 420 nm, and the gap between two contiguous nanocylinders is 200 nm.

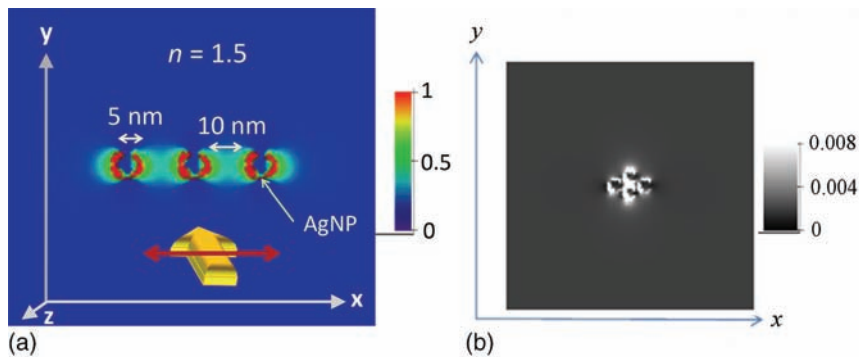


Figure 13.14 Simulation of groups of nanoparticles in three dimensions: (a) linear array of three silver spheres of diameter 5 nm and interparticle distance of 10 nm; (b) cluster of four nanospheres of diameter 5 nm.

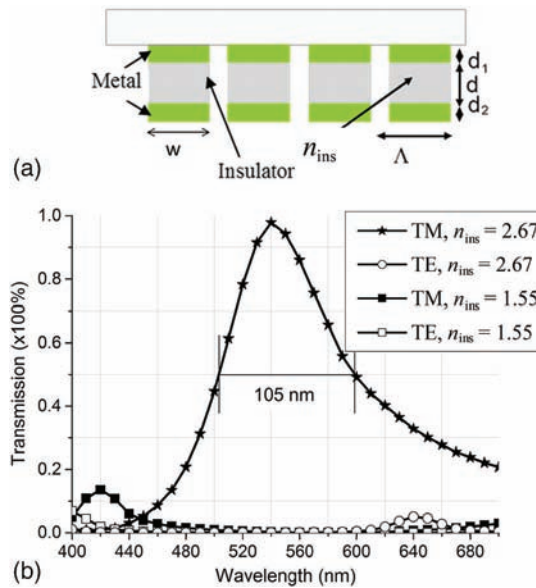


Figure 13.15 (a) Schematic of a composite grating structure;⁴³ (b) transmission spectra in TM and TE modes for the structure with the following structural specifications: $\Lambda = 250$ nm, $d = 100$ nm, $d_1 = d_2 = 40$ nm, $w/\Lambda = 0.7$, and the refractive indices of the insulator layer n_{ins} are 2.67 and 1.55.

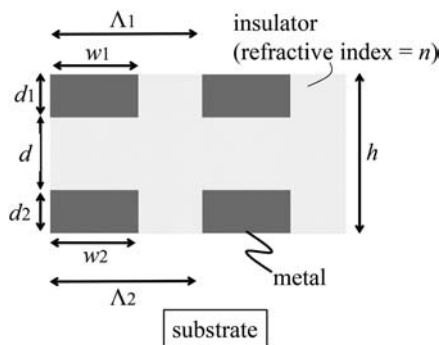


Figure 13.16 Schematic diagram of one of the proposed variations of the structure shown in Fig. 13.15(a). Optical properties depend on values of various design parameters shown in the figure. Λ_1 and Λ_2 are the spatial periods of the first and second composite grating layers, respectively, w_1 and w_2 are the widths of individual grating lines, d_1 and d_2 are the thicknesses of the two metal layers, and d is the thickness of the insulator layer.

In the simulations presented in this section, we terminate the simulation domain on the left and right sides (two sides) along the propagation direction with the first-order nonstandard Mur ABC given by Eq. (13.5). The other two sides (normal to the direction of propagation) of the simulation domain are terminated with a periodic boundary. The gratings and the current sources

extend from one end to the other of the simulation domain. For practical purposes, the periodic boundary conditions on the two sides of the source and the structure emulate a periodic structure that is infinitely repeated in space and in an infinite plane incident wave. A spatial grid resolution h of 4 nm is used in all simulations. The corresponding temporal grid resolution is obtained using Eq. (12.49b).

The real and imaginary parts of the dispersive electrical permittivity of aluminum were obtained from the material handbook.⁴⁶ Two sets of data for the permittivity are plotted in Fig. 13.17. The first set of permittivities comprises the material handbook data interpolated using the cubic spline algorithm (set 1). Since the handbook permittivities are specified at regular frequency intervals, we used cubic spline interpolation to determine the permittivity values at the chosen wavelength sampling points.

The second set of permittivity values in Fig. 13.17 is obtained using a set of best-fit Drude parameters (set 2). The best-fit Drude parameters were computed by fitting the handbook permittivity values to the first-order Drude model [Eq. (12.2)] in the same way as described in Chapter 12. The best-fit Drude parameters are $\hat{\omega}_p = 2.2637 \times 10^{16} \text{ s}^{-1}$ and $\hat{\nu}_c = 11.99 \times 10^{13} \text{ s}^{-1}$. The fitting of the first-order Drude model to the handbook values of permittivities was done over the entire visible domain. In the simulations that follow, the set 2 data obtained with the best-fit Drude parameters are used to determine the aluminum refractive indices.

The transmission properties of the simulated structure depend strongly on the material of the insulator medium. Figures 13.18 and 13.19 show the dependence of transmission spectra in TM and TE modes, respectively, on the

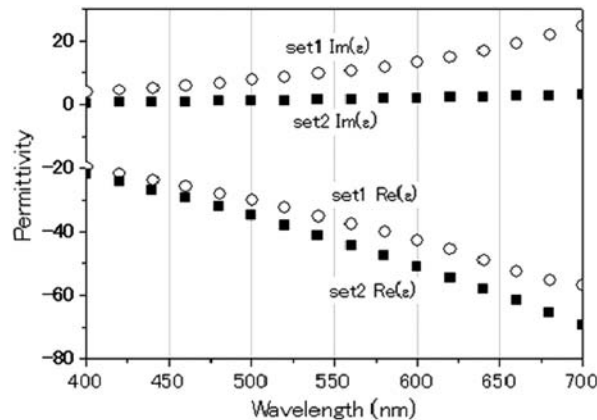


Figure 13.17 Wavelength spectra of two sets of complex permittivities [$\text{Re}(\epsilon)$ is the real part, and $\text{Im}(\epsilon)$ is the imaginary part] of aluminum. Set 1: the handbook permittivities interpolated using the cubic spline algorithm. Set 2: the permittivities obtained using the best-fit Drude parameters. Plasma frequency $= 2.2637 \times 10^{16} \text{ s}^{-1}$, and collision frequency $= 11.99 \times 10^{13} \text{ s}^{-1}$.

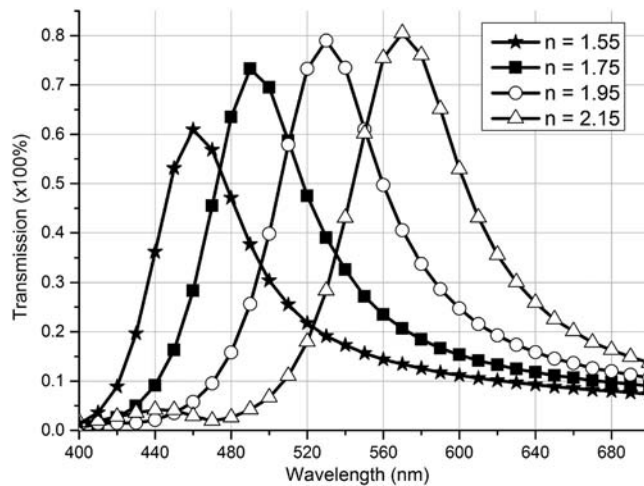


Figure 13.18 Transmission spectra in the TM mode for various values of the refractive index of the insulator layer ($n = 1.55, 1.75, 1.95$, and 2.15). The other structural parameters are: $\Lambda_1 = \Lambda_2 = 250$ nm, $d = 20$ nm, $d_1 = d_2 = 40$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$.

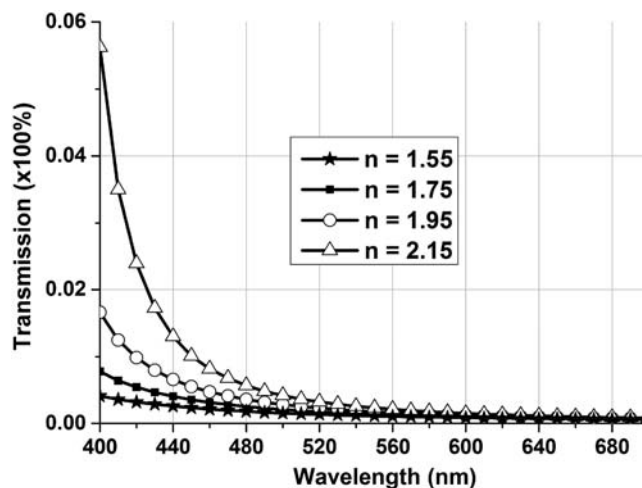


Figure 13.19 Transmission spectra in the TE mode for various values of the refractive index of the insulator layer ($n = 1.55, 1.75, 1.95, 2.15$). The other structural parameters are: $\Lambda_1 = \Lambda_2 = 250$ nm, $d = 20$ nm, $d_1 = d_2 = 40$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$.

refractive index of the insulator layer n . In both cases, the transmission is computed at 10-nm intervals in the 400- to 700-nm wavelength range.

Figure 13.18 shows that the peak transmission in the TM mode increases from 61% for $n = 1.55$ to 76% for $n = 2.15$. The wavelength corresponding to the transmission peak shifts from 460 nm to 570 nm as n increases from 1.55 to 2.15. Also, as n increases from 1.55 to 2.15, the transmission in the TE mode increases rapidly for wavelengths shorter than 440 nm (Fig. 13.19).

From the simulation results presented in Figs. 13.18 and 13.19, it is clear that for the structure shown in Fig. 13.16, a range of $1.55 \leq n \leq 1.95$ is most appropriate. This range ensures above 60% peak transmission in the TM mode and a maximum TE-mode transmission of 21.3% at 400-nm wavelength. When $n > 1.95$, the transmittance in the TE mode for a wavelength of 400 nm can be much larger and reaches up to 48.6% when n becomes 2.15. Such high values of transmittance in the TE mode give rise to an unacceptably small value of the polarization ratio at the corresponding wavelengths.

The results presented in Figs. 13.18 and 13.19 show that the refractive index n of the insulator material is an important design parameter and can be utilized to tune the transmission peak. As n increases, the peak of the transmission spectra in the TM mode shifts toward the longer wavelengths. By increasing n , it is also possible to increase the peak transmission. However, as n increases, the amount of light in undesirable tail bands also increases. Thus, insulator materials with relatively low refractive indices are preferable for this structure.

Figures 13.20 and 13.21 show the transmission spectra in TM and TE modes, respectively, for MIM structures that can be used as blue, green, and red filters. In all three cases, the structure shown in Fig. 13.16 is chosen for simulation. The structural specifications for each case are chosen from the range of parameters suitable for red (R), green (G), and blue (B) filtering. The peak values of transmission in the TM mode are 61%, 86.7%, and 95.1% for B, G, and R filters, respectively. The wavelengths corresponding to the peak

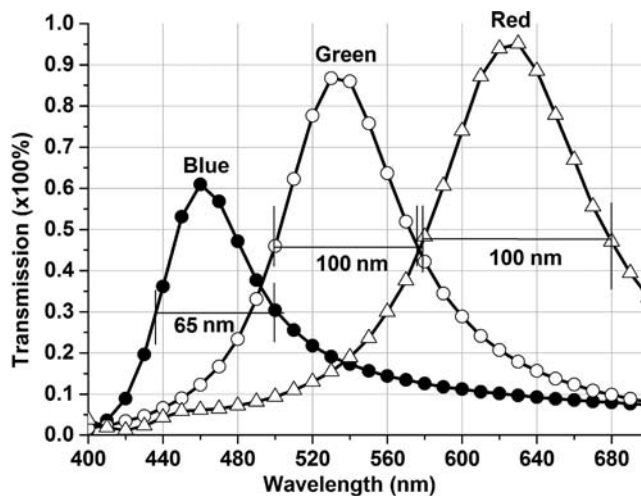


Figure 13.20 Transmission spectra in the TM mode for the structure shown in Fig. 13.16 for three sets of specifications suitable for use as blue, green, and red filters. Blue: $d_1 = d_2 = 40$ nm, $d = 20$ nm, $n = 1.55$, $\Lambda_1 = \Lambda_2 = 250$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$; Green: $d_1 = d_2 = 60$ nm, $d = 20$ nm, $n = 1.55$, $\Lambda_1 = \Lambda_2 = 250$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$; Red: $d_1 = d_2 = 70$ nm, $d = 20$ nm, $n = 1.65$, $\Lambda_1 = \Lambda_2 = 270$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$.

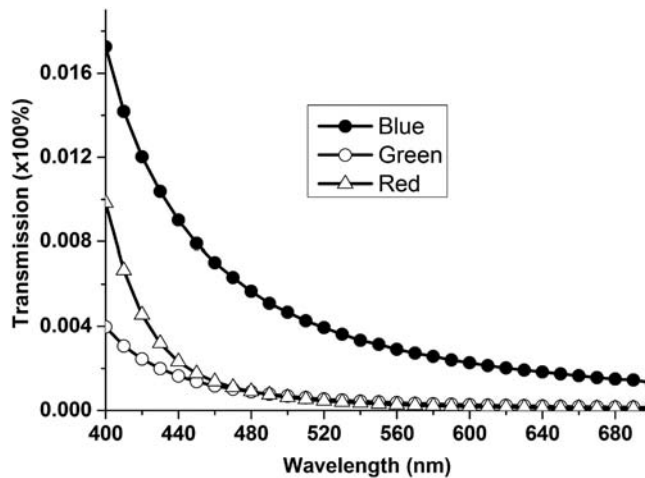


Figure 13.21 Transmission spectra in the TE mode for the structure shown in Fig. 13.16 for three sets of specifications suitable for use as blue, green, and red filters. Blue: $d_1 = d_2 = 40$ nm, $d = 20$ nm, $n = 1.55$, $\Lambda_1 = \Lambda_2 = 250$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$; Green: $d_1 = d_2 = 60$ nm, $d = 20$ nm, $n = 1.55$, $\Lambda_1 = \Lambda_2 = 250$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$; Red: $d_1 = d_2 = 70$ nm, $d = 20$ nm, $n = 1.65$, $\Lambda_1 = \Lambda_2 = 270$ nm, and $w_1/\Lambda_1 = w_2/\Lambda_2 = 0.7$.

transmissions are 460 nm, 535 nm, and 630 nm for B, G, and R filters, respectively. The FWHM is 100 nm for both the G and R filters. The maximum transmission in the TE mode is 1.8% at a wavelength of 400 nm for the B filter. The maximum transmissions in the TE mode are 0.4% and 0.98% for G and R filters, respectively. In all three cases, the polarization ratio can be quite high (above 0.97) at the peak transmission wavelengths. The polarization ratio is the lowest in the case of the blue filter.

Figures 13.22(a) and (b) show the simulated intensity distribution of light inside the structure shown in Fig. 13.16 at two different wavelengths. The dimensions of various parameters of the structure are as follows: $d = 20$ nm, $\Lambda_1 = \Lambda_2 = 250$ nm, $d_1 = d_2 = 40$ nm, and $n = 1.55$. The color bar shows the scale to which the intensity is plotted. Figure 13.22(a) corresponds to the peak

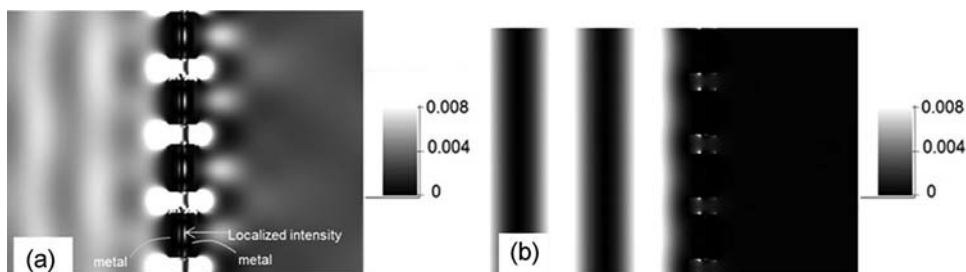


Figure 13.22 (a) Intensity distribution of light inside the structure shown in Fig. 13.16 at (a) $\lambda = 460$ nm and (b) $\lambda = 700$ nm. The structural specifications are the same as those of the blue filter in Fig. 13.20.

transmission wavelength at 460 nm. Figure 13.22(b) corresponds to a wavelength of 700 nm when the transmission is low. Figure 13.22(a) clearly shows a localization and enhancement of light intensity at the two boundaries between the metal and the insulator layer. This phenomenon is a clear indication of generation of LSPR modes. In contrast, Fig. 13.22(b) does not show any localization or enhancement at the metal–insulator interfaces. Hence, Figs. 13.22(a) and (b) establish a clear relation between the LSPR modes and the peak transmission. Therefore, we conclude that the color-filtering behavior of the MIM structures discussed here can be associated with plasmon-related resonances.

The peak value of transmission can be increased by reducing the separation d between the two metal grating layers. However, peak transmission wavelength does not vary much, even when the value of d changes significantly.

Additional simulations indicate that the thicknesses of the first and second metal grating layers can be adjusted in order to tune the wavelengths corresponding to the peak transmission. We also found that for acceptable performance, the periods of the first and second metal grating layers should be ≥ 230 nm and ≤ 270 nm.

13.3 Summary

In this chapter we discuss the results of simulating scattering of light by pairs, arrays, and clusters of silver nanocylinders. The simulations were carried out using the MRC-FDTD methodology described in Chapter 12 in two and three dimensions. Extinction spectra are computed in the TM mode for various pairs of nanocylinders. The simulations indicate that the position and size of the peaks of the extinction spectra are determined by the distance between the two cylinders. The LSPR peak can be shifted toward the longer wavelengths (red-shift) by reducing the interparticle distance. The red-shift increases as the interparticle distance becomes smaller. The results show that the red-shift of the extinction peak occurs as the gap between the cylinders is reduced when the incident light is polarized in a direction parallel to the gap between the cylinders. In contrast, when the direction of polarization of the incident light is normal to the gap, the extinction peak cannot be moved by bringing the cylinders closer to each other.

As a second example of simulations using MRC-FDTD, we discuss the design and simulation of a MIM-based nanoresonator structure that can show color-filter-like transmission and useful polarization properties. The simulation results indicate that it might be possible to implement the structure using low-refractive-index insulator materials. This possibility can lead to the use of polymeric or organic materials that are inexpensive compared to inorganic semiconductor materials. The performance of such a structure can also be

much better than that of conventional, dye-based color filters. Simulations show that the bandwidths of transmission for blue, green, and red filters can be less than 100 nm, and minimum peak transmission can be above 60%. The peak transmission is lowest for the blue filters and increases for filters operating at longer wavelengths.

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Chapter 14

Photonics Design

In this chapter we discuss design processes of two photonic structures. Both examples involve multilayer structures that are common in optics and photonics. In engineering and industrial applications, design issues of these structures are commonly encountered. The design processes described here illustrate the need for combining other numerical methods with FDTD. In Section 14.1, a systematic design process is discussed that starts with an *ab initio* design phase based on effective medium theory. In Section 14.2, a second example is discussed, in which a global optimization scheme based on a genetic algorithm is combined with the analytical characteristic matrix approach for a thin film stack made up of isotropic and anisotropic materials. Both structures are designed for application in liquid crystal displays (LCDs).

Topics:

- Designing low-reflection, multilayer wire-grid polarizers
- Designing wavelength-selective, polarizing reflector films

14.1 Designing Low-Reflection, Multilayer Wire-Grid Polarizers for LCD Applications

Wire-grid polarizers (WGP) are studied extensively for application in LCD devices.^{1–8} WGP are zero-order, subwavelength metal gratings and are highly efficient polarizers. When a WGP is illuminated with unpolarized light, it transmits the TM polarized component (electric field perpendicular to the grating ridges) and reflects the TE component (electric field parallel to the grating ridges). In applications such as projection displays, the reflected light from conventional WGP can cause ghost images to form. These ghost images are caused by the stray light that is not directed through the projection optical unit to the nominal image plane, but which instead gets diffused by multiple reflections from the partially refractive surfaces of various optical components.⁹ This unwanted light causes glare and leads to significant loss of contrast, light leakage in the dark state, heat generation, and concomitant deterioration of

image quality. Hence, when using a WGP, it is necessary to reduce the amount of light that is reflected from its surface. A reflection-suppressing, bilayer design of a WGP is proposed in Ref. 10.

In general, the WGP structures proposed to date for suppressing reflection are complicated, requiring multiple layers. Such designs, while effective in reducing reflection over a broadband of wavelengths, might be too expensive to fabricate for most display applications. When we embarked on the design of multilayer WGP, one of our goals was to study simpler structures comprising fewer layers that might be less expensive to fabricate. Accordingly, we looked at designs of WGP involving just two or three layers. Reducing the number of layers alone cannot guarantee low fabrication cost unless the materials of the coating layers and the fabrication process are carefully chosen. Electron beam evaporation or sputtering, which allows the designer to choose from a wide spectrum of materials, might be appropriate as a fabrication process.¹¹

In this chapter, we develop a systematic approach to the design of multilayer WGP. We investigate the relation between the refractive indices of the additional layers and the reflection in the TE mode. From simulations, we found that adding just one or two thin layers of suitably chosen semiconductors on top of the metal ridges of an ordinary metallic WGP is sufficient to appreciably lower the reflection in a specified band of wavelengths. Such a simple structure can have some practical applications. The design method is discussed here as an illustrative example and can be extended to solve other problems, especially those involving periodic structures.

As is evident from the references reviewed here, various computational techniques have been employed in the design and simulation of WGP. In Ref. 2, finite-aperture WGP are simulated using the 3D FDTD method implementing the Lorentz model of electric permittivity. Metallic waveguide theory and the finite element method have been used to design WGP meant for liquid crystal on silicon (LCoS) systems.⁵ References 6 and 7 use a modal analysis and a differential theory of diffraction gratings, respectively, to simulate WGP used in LCoS microdisplays. In Ref. 12, recursive, stable matrix algorithms are developed for multilayer grating simulations.

We developed a design method involving an *ab initio* phase.¹³ In this phase of design, an effective medium theory (EMT) for gratings¹⁴ is employed in combination with the characteristic matrix method for multilayers of thin films.¹⁵ This phase is quick and effectively identifies suitable layer materials.

However, the EMT approach can only yield approximate results. Since the multilayer WGP considered here employ subwavelength feature sizes, we need to solve Maxwell's equations to accurately compute the diffraction properties. Hence, in the final phase of the design process, we use an FDTD algorithm to compute the polarization-dependent reflection and transmission spectra for the actual structure. The FDTD program used in this chapter

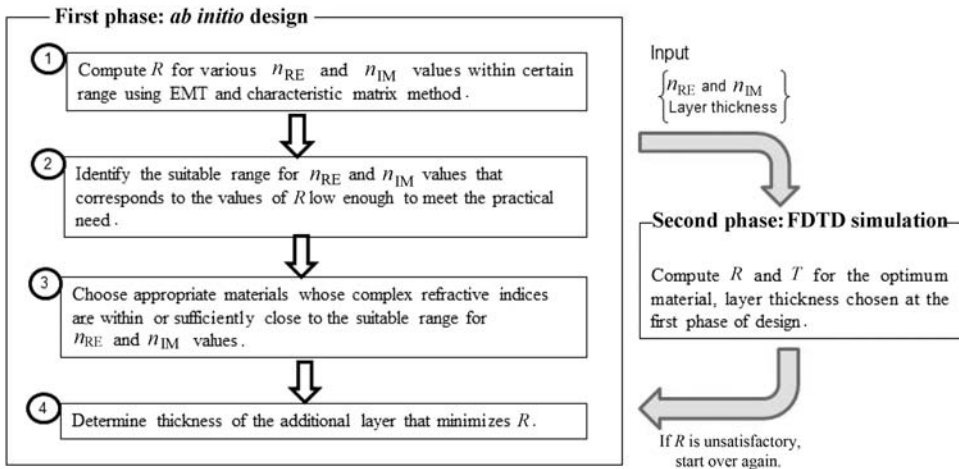


Figure 14.1 Design flowchart consisting of two phases: *ab initio* design and FDTD simulation. n_{RE} and n_{IM} are the real and imaginary parts, respectively, of the complex refractive index of the material of the additional layer, R is the reflection coefficient, and T is the transmission coefficient.

employs dielectric FDTD to simulate the lossy dielectric layers and the MRC-FDTD method (developed in Chapter 12) to simulate the metal layers of the multilayer WGP. Figure 14.1 is a flowchart representing the process used to design the multilayer WGP.

Figure 14.2 is a schematic diagram of vertical cross-sections of an ordinary and a bilayer WGP. The material of the ridges in the ordinary WGP is aluminum. The bilayer structure contains one metallic part that is structurally the same as the ordinary WGP. Various structure-related design parameters are indicated in the figure: Λ is the period of the ridges, and w is the width of an individual ridge of the ordinary and bilayer WGP. For all of the simulations in this section, $\Lambda = 155$ nm, $f = 0.3$, ridge height $d = 200$ nm,

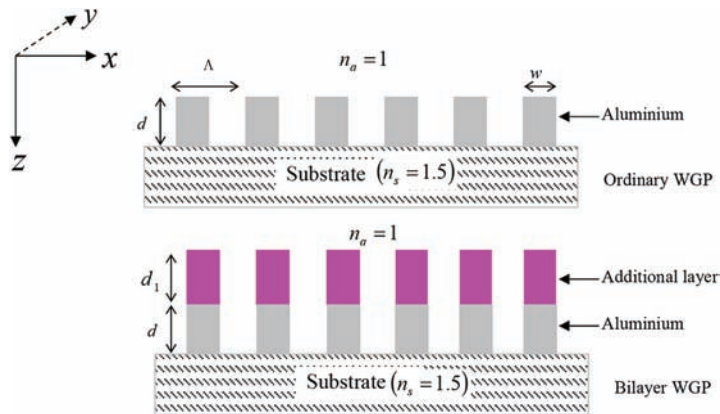


Figure 14.2 Cross-sectional view of an ordinary (top) and a bilayer (bottom) WGP. The structural design parameters are indicated.

and d_1 is the thickness of the additional layer and is treated as a variable. All of the simulations were carried out for normal incidence (light incident along the z axis). In all cases, the refractive index of the substrate $n_s = 1.5$, and the refractive index of the incident medium $n_a = 1$.

In the following sections the *ab initio* design methods and the results of simulations obtained using *ab initio* design and FDTD are presented.

14.1.1 *Ab initio* design

In this phase, we approximate the multilayer WGP by a stack of thin film layers, where each thin film layer has an effective refractive index. The effective refractive index of each layer is estimated using a zero-order EMT for subwavelength gratings. The effective refractive indices in TE and TM modes are given by

$$\eta_{\text{TE}} = \left[n_m^2 f + n_g^2 (1 - f) \right]^{1/2}, \quad (14.1)$$

$$\eta_{\text{TM}} = \left[\frac{f}{n_m^2} + \frac{(1 - f)}{n_g^2} \right]^{-1/2}. \quad (14.2)$$

In Eqs. (14.1) and (14.2), n_m is the refractive index of metals or semiconductors forming the grating ridges, and n_g is the refractive index of the material separating any two consecutive ridges. f is the fill factor and is given by

$$f = w/\Lambda, \quad (14.3)$$

where Λ is the spatial period of the WGP, and w is the width of an individual ridge of the WGP.

As described in Chapter 12, the reflection and transmission coefficients of a multilayer consisting of thin films can be computed using the characteristic matrix method.¹⁵ The characteristic matrix $\mathbf{M}$ of the multilayer is given by

$$\mathbf{M} = \prod_j \mathbf{m}_j, \quad (14.4)$$

where

$$\mathbf{m}_j = \begin{bmatrix} \cos \beta_j & (-i/\eta_j) \sin \beta_j \\ -i\eta_j \sin \beta_j & \cos \beta_j \end{bmatrix}. \quad (14.5)$$

For normal incidence, $\beta_j = \eta_j t_j (2\pi/\lambda)$, where η_j is the effective complex refractive index obtained from Eqs. (14.1) and (14.2), t_j is the thickness (length along the propagation direction of light) of the j^{th} layer, and λ is the incident wavelength of light. Since the effective refractive indices are different for TE and TM modes, the values of β_j are also different for these two modes.

The overall reflection coefficient (the intensity of the reflected light expressed as a fraction of the intensity of incident light) of a bilayer WGP in TE mode is given by [same as Eq. (12.90)]

$$R = \left| \frac{(M_{1,1} + M_{1,2}n_s)n_a - (M_{2,1} + M_{2,2}n_s)}{(M_{1,1} + M_{1,2}n_s)n_a + (M_{2,1} + M_{2,2}n_s)} \right|^2, \quad (14.6)$$

where the different elements of M are computed using Eq. (14.4), and n_a and n_s are the refractive indices of the incident medium and of the substrate, respectively.

Using Eq. (14.6), we compute the reflection coefficient of a bilayer WGP in the TE mode as a function of the real and imaginary parts of the refractive index of the material of the additional layer. The real part of the refractive index n_{RE} is varied within the range of 1.5 to 6.5 in increments of 0.2; for each value of n_{RE} , the imaginary part of the refractive index n_{IM} , is varied from 0.01 to 2.51 in increments of 0.1. The reflection coefficient is computed at each (n_{RE}, n_{IM}) point and plotted as a contour map in Fig. 14.3. The wavelength λ of the incident light is 460 nm, and $d_1 = 20$ nm. For the simulations, we used handbook permittivity values (data set 1 in Fig. 13.17) to determine the refractive indices of aluminum. The results are presented in Fig. 14.3, which shows that for a bilayer WGP, the value of the reflection coefficient depends on the complex refractive index of the material of the additional layer. The lowest values of the reflection coefficient are associated with the relatively large values of n_{RE} and n_{IM} of the additional layer. The desirable ranges for n_{RE} and n_{IM} are $4.5 \leq n_{RE} \leq 5.5$

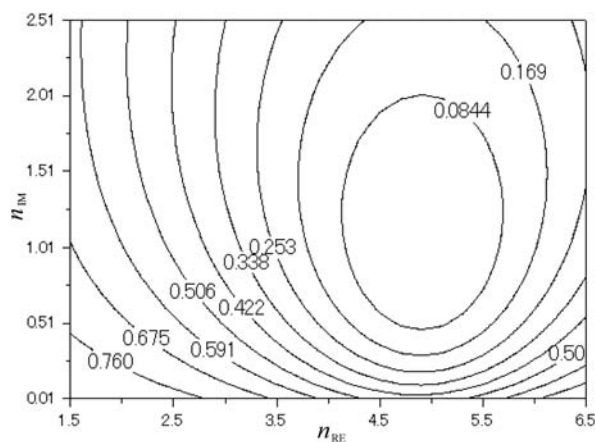


Figure 14.3 Contour map of the reflection coefficient of a bilayer WGP plotted as a function of the real (n_{RE}) and imaginary (n_{IM}) parts of the refractive index of the additional layer at wavelength $\lambda = 460$ nm. The structural specifications for the WGP are $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

and $0.51 \leq n_{\text{IM}} \leq 2.01$, respectively. Figure 14.3 also shows that an arbitrary choice of material for the additional layer might not be very effective in reducing the reflection.

The desirable ranges for n_{RE} and n_{IM} change when the wavelength of the incident light changes. In Fig. 14.4, we plot the reflection coefficient in the TE mode as a function of the real and imaginary parts of the refractive index of the material of the additional layer at $\lambda = 540$ nm. The other parameters are same as in Fig. 14.3.

Comparing Fig. 14.3 with Fig. 14.4, we find that the region of minimum reflection shifts laterally toward the right as λ increases. Hence, at longer wavelengths, materials with larger n_{RE} values (≈ 5 –6.5) need to be used for the additional layer.

Semiconductors such as silicon or gallium arsenide show relatively large n_{RE} values in the visible domain. For silicon, n_{RE} varies approximately from 3.6 to 5.6, while for gallium arsenide, n_{RE} varies approximately from 3.6 to 4.5.¹⁶ For silicon, n_{IM} varies approximately from 0.01 to 0.39, while for gallium arsenide, n_{IM} varies approximately from 0.14 to 2.2.¹⁶ Thus, with silicon or gallium arsenide as the material for the additional layer, we expect about 60% or 90%, respectively, reduction in reflection around $\lambda = 460$ nm. However, since the complex refractive indices of both silicon and gallium arsenide vary significantly with wavelength, we can only expect such a large reduction in reflection over a narrow band of wavelengths around 460 nm. Hence, in the computational examples that follow, we use silicon and gallium arsenide as the materials for the additional layer.

Next, the reflection coefficients of the two bilayer WGs in the TE mode are computed as function of the thickness of the additional layer d_1 .

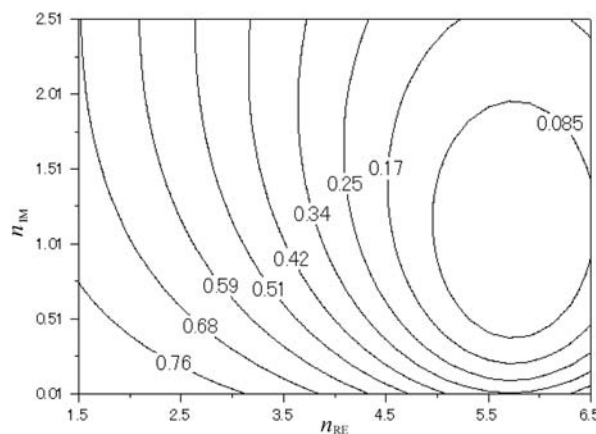


Figure 14.4 Contour map of the reflection coefficient of a bilayer WGP plotted as a function of the real (n_{RE}) and imaginary (n_{IM}) parts of the refractive index of the additional layer at $\lambda = 540$ nm. The structural specifications for the WGs are $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

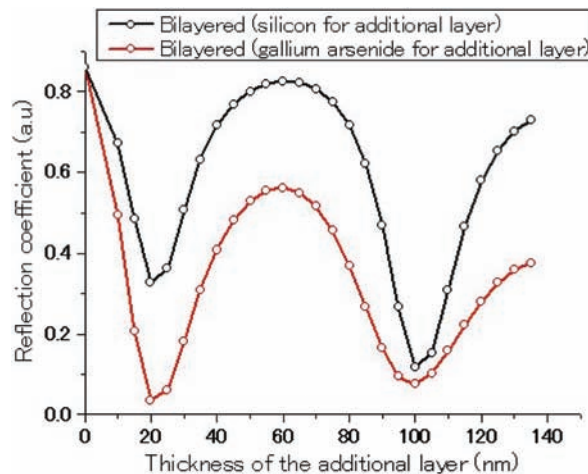


Figure 14.5 Reflection coefficients of the bilayer WGPs plotted as functions of the thickness of the additional layer d_1 at $\lambda = 460$ nm. The materials of the additional layer are silicon (black) and gallium arsenide (red). The structural specifications for the WGPs are $\Lambda = 155$ nm, $d = 200$ nm, and $f = 0.3$.

The results are plotted in Fig. 14.5, which indicates a strong dependence of reflection coefficient on the thickness of the additional layer for the chosen materials. In both cases, minima in reflection coefficients occur at $d_1 = 20$ nm. For these computations, $\lambda = 460$ nm. Thus, we choose $d_1 = 20$ nm for the additional layer for both of the bilayer WGPs. The wavelength spectra of reflection coefficients for the ordinary and bilayer WGPs are computed in Section 14.1.2.

14.1.2 Results

In this section we compute the diffraction properties in both the forward (transmission) and backward (reflection) directions of the ordinary and the two bilayer WGPs using both *ab initio* design techniques and FDTD algorithm. The WGPs considered are periodic along one direction, finite along a perpendicular direction, and structurally invariant along the third, orthogonal direction. Due to this structural symmetry, the WGPs are simulated in two dimensions.

Ab initio design

The wavelength spectra of reflection coefficients for the ordinary and the two bilayer WGPs are computed in the TE mode. The results are plotted in Fig. 14.6. These approximate results indicate that the two simulated bilayer WGPs can be used as low-reflection WGPs, particularly for wavelengths around 440 nm.

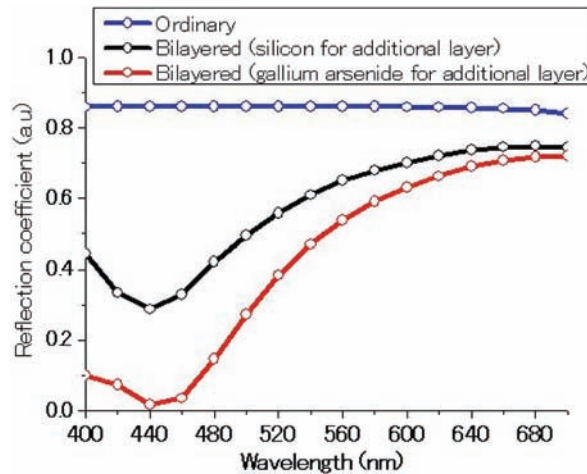


Figure 14.6 TE-mode reflection spectra computed using *ab initio* design methods; blue is the ordinary WGP, black is the bilayer WGP (silicon for additional layer), and red is the bilayer WGP (gallium arsenide for the additional layer). The structural specifications for the WGP are $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

FDTD

Figures 14.7–14.10 show the wavelength spectra of reflection and transmission in both TE and TM modes for the ordinary WGP and the two bilayer WGPs computed using FDTD. The material of the ridges of the ordinary WGP is aluminum. In the case of the bilayer WGPs, the additional layer is

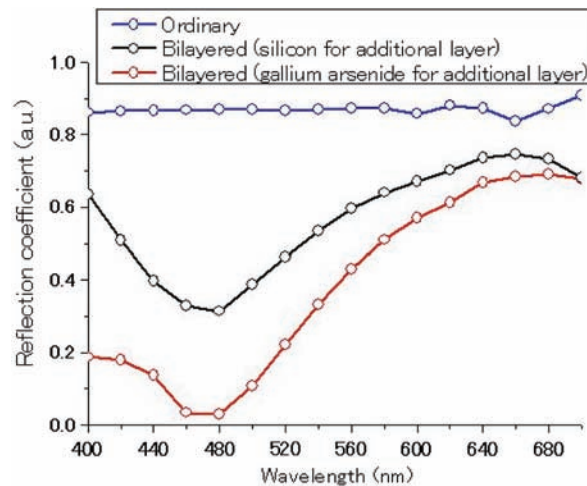


Figure 14.7 Reflection spectra for the ordinary WGP (blue) and the two bilayer WGPs (black and red) in the TE mode computed using FDTD. In the case of the bilayer WGPs, the materials used for the additional layers are silicon (black) and gallium arsenide (red). The structural specifications for the WGP are $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

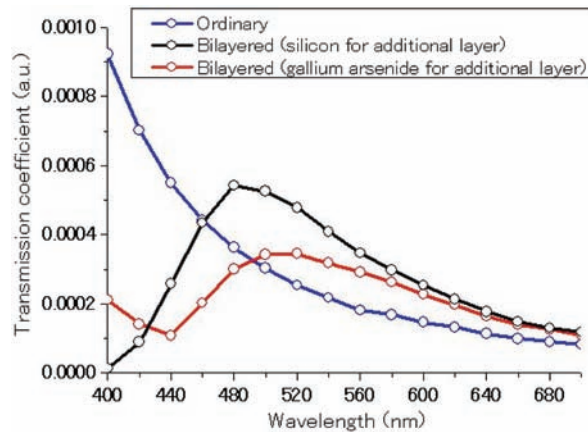


Figure 14.8 Transmission spectra for the ordinary WGP (blue) and the two bilayer WGPs (black and red) in the TE mode computed using FDTD. In the case of the bilayer WGPs, the materials used for the additional layers are silicon (black) and gallium arsenide (red). The structural specifications for the WGPs are $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

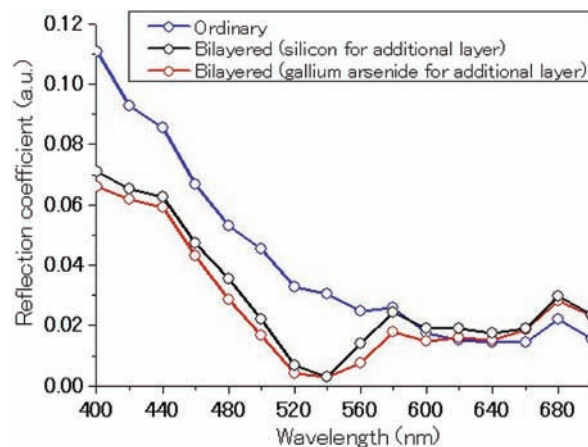


Figure 14.9 Reflection spectra for the ordinary WGP (blue) and the two bilayer WGPs (black and red) in the TM mode computed using FDTD. In the case of the bilayer WGPs, the materials used for the additional layers are silicon (black) and gallium arsenide (red). The structural specifications for the WGPs are $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

either silicon or gallium arsenide. All three WGPs have the following structural specifications: $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

The reflection and transmission coefficients are computed from the reflected and transmitted irradiance (radiant flux per unit area) data sampled at grid points close to the last interface of the WGP structure. The results presented in Figs. 14.7–14.10 are computed using the following simulation parameters: minimum space step or grid resolution $h = 4$ nm, minimum time step $\Delta t = 1.33 \times 10^{-18}$ s, and $\nu = 0.1$.

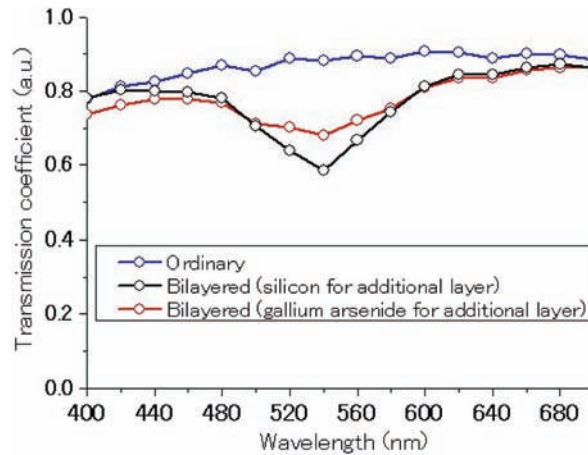


Figure 14.10 Transmission spectra for the ordinary WGP (blue) and the two bilayer WGs (black and red) in the TM mode computed using FDTD. In the case of the bilayer WGs, the materials used for the additional layers are silicon (black) and gallium arsenide (red). The structural specifications for the WGs are $\Lambda = 155$ nm, $d = 200$ nm, $f = 0.3$, and $d_1 = 20$ nm.

14.1.3 Discussion

We used the design process described in Sections 14.1.1 and 14.1.2 to design low-reflection, bilayer WGs. The goal of the design process is to identify materials and thicknesses for the additional layers that are effective in reducing the reflection of the WGs. Simulations also indicate that such modifications of ordinary WGs brought about by adding extra layers do not affect their high polarization efficiency. However, the transmission in the TM mode can diminish by as much as 25% for a narrow band of wavelengths.

Even the approximate computations (Fig. 14.6) in the *ab initio* phase of design can effectively identify the materials of the additional layers. This phase is useful because the results are obtained quickly.

Both the approximate (Fig. 14.6) and the rigorous (Fig. 14.7) results suggest that simple, bilayer WGs might be good for practical applications seeking low-reflection WGs. The bilayer design of WGs is particularly effective if the low-reflection behavior is expected over a narrow band of wavelengths. The key is the appropriate choice of material and the thickness of the additional layer. By adding a layer with suitable optical properties to the ordinary WGP, the reflection can be lowered to a desired level within a certain predetermined band of wavelengths. The amount by which the reflection can be lowered depends on the values of the real and imaginary parts of the refractive indices of the material of the additional layer. For example, gallium arsenide is more effective in lowering reflection compared to silicon for the same band of wavelengths. It is also possible to widen the wavelength band of operation for WGs by adding extra layers.

We have explored the dependence of TE-mode reflection on the real and imaginary parts of the refractive index of the material of the additional layer using approximate design methods. It appears that at any particular wavelength, TE-mode reflection reaches a minimum for a certain range of values of the complex refractive index of the layer material. The plot of the TE-mode reflection coefficient versus real and imaginary parts of the refractive index of the material of the additional layer (Figs. 14.3 and 14.4) allow us to find a real material for the layer. Hence, the design process introduced here can be used to guide a search for a suitable material for the additional layer. This would simplify the design process of an actual device, eliminating the need to arbitrarily fix the structural parameters. For the sake of simplicity, the design principle is explained here using a bilayer WGP. The same principle can also be used to design a multilayer WGP that contains more than two layers.

Thus, the simulation results point to the existence of simpler, more cost-effective structures (bilayer versus multilayer) for low-reflection WGP. The appropriate choice of layer material can also lead to a simpler fabrication process.

As expected, the results of approximate (Fig. 14.6) and rigorous (Fig. 14.7) computations are different. The approximate computations show that reflectivity becomes a minimum at or around a wavelength of 440 nm, whereas, the rigorous FDTD computations indicate that the minimum reflectivity occurs between 460 nm and 480 nm. However, both computations confirm the low-reflection behavior of WGP.

14.2 Designing Wavelength-Selective, Polarizing Reflector Films for LCD Applications

Multilayer plastic films capable of showing iridescent colors have been developed for display purposes.¹⁷

In particular, recently, multilayer reflector films have been designed and developed for broad-wavelength-band,¹⁸ broad-angular-range applications.¹⁹ Such films are commonly used in LCDs to increase the overall brightness.

Typically, such multilayer films are composed of hundreds of coextruded thin layers of polymer. The thickness of any individual layer is less than the wavelength of visible light, typically less than 200 nm. The multilayer is a periodic or quasi-periodic structure formed by repeating one basic unit containing two layers of two different materials (say, A and B). Layers A and B are chosen from transparent, nonabsorbing polymers. In the case of polarizing reflectors, one of the layers (say, A) is optically isotropic, while the other layer is uniaxially birefringent. Such films are highly reflective in one polarization mode and are highly transmissive in the orthogonal polarization mode.

Many methods are available for the design of thin film multilayers.²⁰ In recent years, automatic design methods based on local and global optimization

techniques attracted much attention. Various authors have used evolutionary algorithms and global optimization techniques to design multilayers possessing uniformly high reflectivity over a broad range of angles,^{21,22} antireflection properties for infrared wavelengths,²³ high reflectivity over a narrow band of wavelengths,^{24,25} and high reflectivity in extreme-ultraviolet light.²⁵

Here, we discuss the design process of a multilayer film²⁶ that can function as a wavelength-selective polarizing reflector (WSPR). Such films can be used in LCDs to enhance the color saturation of the device.

A combination of a characteristic matrix method and a version of genetic algorithm (GA) is used to design the multilayer WSPR film. The refractive indices and thicknesses of layers A and B are determined such that the reflectivity spectrum in one polarization mode matches a pre-specified target spectrum.

In the subsections that follow, the design method, the results involving the optimization of the multilayer structure, the computation of the reflectivity spectra, and the proposed application of the same in LCD devices are described.

14.2.1 Method of design

Figure 14.11 shows the basic unit of the multilayer consisting of two layers A and B. The principal refractive indices of layers A and B are nA_x , nA_y , nA_z and nB_x , nB_y , nB_z , respectively; tA and tB are the thicknesses of the layers A and B, respectively. We consider the case of normal incidence, where the incident and transmitted light propagate along the y axis, while reflected light propagates along the $-y$ axis. To simulate an anisotropic medium in two dimensions, we assume the principal axes to be aligned with our chosen coordinate system.

Characteristic matrix

We compute the reflection and transmission properties of the thin film stack using the characteristic matrix method.¹⁵ The characteristic matrix $\mathbf{M}_{AB}$ for

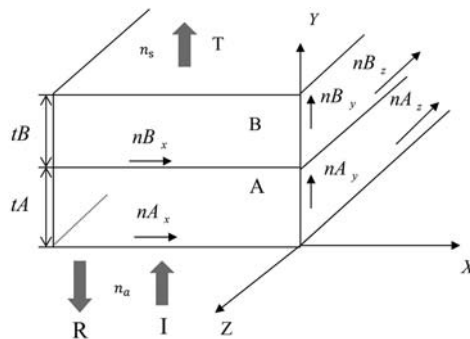


Figure 14.11 Basic structural unit of a multilayer consisting of layers A and B. The directions of incident, reflected, and transmitted light are indicated with the letters I, R, and T, respectively.

the basic unit (consisting of a layer of material A stacked on top of a layer of material B), as shown in Fig. 14.11, is given by¹⁵

$$\mathbf{M}_{AB} = \mathbf{M}_A \mathbf{M}_B, \quad (14.7)$$

where $\mathbf{M}_A$ and $\mathbf{M}_B$ are the characteristic matrices for layers A and B, respectively. $\mathbf{M}_A$ and $\mathbf{M}_B$ are determined by the admittances αA , αB of layers A and B, respectively. In TE (electric field normal to the plane of incidence x - y) and TM (electric field in the plane of incidence x - y) modes, for normal incidence, αA and αB are given by¹⁵

$$\alpha A_{\text{TE}} = nA_z, \quad (14.8a)$$

$$\alpha B_{\text{TE}} = nB_z, \quad (14.8b)$$

$$\alpha A_{\text{TM}} = nA_x, \quad (14.9a)$$

$$\alpha B_{\text{TM}} = nB_x. \quad (14.9b)$$

The optical phases βA and βB of layers A and B are given by

$$\beta A_{\text{TE}} = \left(\frac{2\pi}{\lambda} \right) \cdot \alpha A_{\text{TE}} \cdot tA, \quad (14.10a)$$

$$\beta B_{\text{TE}} = \left(\frac{2\pi}{\lambda} \right) \cdot \alpha B_{\text{TE}} \cdot tB, \quad (14.10b)$$

$$\beta A_{\text{TM}} = \left(\frac{2\pi}{\lambda} \right) \cdot \alpha A_{\text{TM}} \cdot tA, \quad (14.11a)$$

$$\beta B_{\text{TM}} = \left(\frac{2\pi}{\lambda} \right) \cdot \alpha B_{\text{TM}} \cdot tB. \quad (14.11b)$$

The condition for constructive interference for the pair of layers shown in Fig. 14.11 is given by

$$\beta A + \beta B = q \pi \lambda, \quad (14.12)$$

where q is an odd number. If Eq. (14.12) is satisfied at a certain wavelength λ , the corresponding reflectivity reaches a maximum.

In the TE mode, M_A and M_B are given by¹⁵

$$M_A = \begin{bmatrix} \cos(\beta A_{\text{TE}}) & -\frac{i}{\alpha A_{\text{TE}}} \sin(\beta A_{\text{TE}}) \\ -i \cdot \alpha A_{\text{TE}} \cdot \sin(\beta A_{\text{TE}}) & \cos(\beta A_{\text{TE}}) \end{bmatrix}, \quad (14.13)$$

$$M_B = \begin{bmatrix} \cos(\beta B_{TE}) & -\frac{i}{\alpha B_{TE}} \sin(\beta B_{TE}) \\ -i \cdot \alpha B_{TE} \cdot \sin(\beta B_{TE}) & \cos(\beta B_{TE}) \end{bmatrix}. \quad (14.14)$$

In the TM mode, M_A and M_B are obtained by replacing α and β , respectively, with their counterparts in the TM mode.

For a stack consisting of N basic units (layer A + layer B), the characteristic matrix $\mathbf{M}$ is given by

$$\mathbf{M} = (\mathbf{M}_{AB})^N. \quad (14.15)$$

The elements of $\mathbf{M}$ computed from Eq. (14.15) are used in Eq. (14.6) to compute the reflectivity of the stack. Recall that n_a and n_s in Eq. (14.6) are the refractive indices of the incident and the emergent (substrate) media, respectively.

Optimization

The issue of designing the multilayer film is formulated as a constrained optimization problem. The performance of a multilayer is estimated in terms of the difference between the reflectivity spectrum of the multilayer and a pre-specified target spectrum. A merit function ϕ is defined to measure this difference and is given by

$$\phi = \frac{1}{N_\lambda} \sum_{j=1}^{N_\lambda} (R_j - \rho_j)^2, \quad (14.16)$$

where N_λ is the total number of wavelength sampling points, R_j is the reflectivity of the multilayer at the wavelength sampling point λ_j , and ρ_j is the target reflectivity at λ_j . Here, N_λ is 60 (interval = 5 nm) in the wavelength range [400 nm, 700 nm].

The merit function ϕ is minimized using a genetic algorithm (GA) method, which is a stochastic intelligent search method. The input is a population of randomly generated candidate solutions, each of which represents a multilayer structure. The solutions are updated through a given number of generations by applying various operators that roughly mimic the natural evolution process. The evolution process is implemented with the help of operators such as tournament selection, uniform crossover, and bit mutation.²⁷ Apart from these three major operators, a measure of genetic diversity is introduced to ensure sufficient diversity in the population as it progresses through newer generations. This prevents stagnation around a local optimum. A speciation scheme is incorporated in order to be able to identify a number of local minima as well as the global minimum. Brief descriptions of the major operators are provided below.

Design variables

The design variables are nA_x , $\Delta n (= nB_x - nA_x)$, and the six layer thicknesses for the three basic units corresponding to three stacks, e.g., tA_1 , tB_1 , tA_2 , tB_2 , tA_3 , and tB_3 . The ranges for the first two variables are $[1.45, 2]$ and $[0.0, 0.15]$, respectively. For the thickness variables, the range is chosen to be the same, e.g., $[5 \text{ nm}, 205 \text{ nm}]$.

Binary coding of variables

Each design variable is represented as a fixed-length binary substring of 0s and 1s. When decoded, any binary substring s of length l converts to a specific value of the design variable x . This value of x is given by

$$x = x_{\min} + \frac{x_{\max} - x_{\min}}{2^l - 1} DV(s), \quad (14.17)$$

where $x_{\max}$ and $x_{\min}$ are the maximum and minimum allowed values of x , $DV(s)$ represents the decoded decimal equivalent of s , and l is decided by the minimum step allowed in the respective variable.

The structure of any particular multilayer is specified by a binary string S , which is generated by combining the substrings representing all of the design variables. S is given by

$$S = s_\nu s_{\nu-1} \cdots s_0, \quad (14.18)$$

where ν is the number of variables, and $\nu = 8$. The right side of Eq. (14.18) does not represent a multiplication but simply indicates the process of forming a longer string by positioning the individual substrings next to each other. The resulting string on the right side of Eq. (14.18) encodes all of the design variables.

Tournament selection

The tournament selection operator mimics the process of mate selection observed in nature. The fittest among a set of randomly chosen solutions are selected to a mating pool with a preassigned probability p_t .

Uniform crossover

The uniform crossover operator effectively explores the design space. A pair of bit strings is selected from the mating pool with a probability p_c . A next-generation bit string is created from the two parent bit strings by combining bits from each according to a randomly generated crossover mask.

Bit mutation

The bit mutation operator facilitates local search. It randomly alters each bit of the bit string with a small probability p_m .

14.2.2 Multilayer films

The target spectrum is constructed by adding the emission spectra of the red, green, and blue LEDs, and shows three peaks at approximately $\lambda_B = 462.5$ nm, $\lambda_G = 532.5$ nm, and $\lambda_R = 632.5$ nm. In keeping with the three peaks of the target spectrum, the solution is sought among populations of three-stack multilayers.

We set A as an isotropic layer and B as a uniaxially birefringent layer. A and B are chosen in a way that ensures the following relationship among the refractive indices:

$$nA_x = nA_y = nA_z = nB_y = nB_z \neq nB_x. \quad (14.19)$$

All three basic units of the three stacks use layers A and B, albeit, with differing thicknesses.

Figure 14.12 shows the target spectrum and the reflectivity spectra of an optimized multilayer in TE and TM modes. The optimum solution is: $nA_x = 1.6097$, $\Delta n = 0.1$, $tA_1 = 117.07$ nm, $tB_1 = 74.17$ nm, $tA_2 = 49.48$ nm, $tB_2 = 89.36$ nm, $tA_3 = 79.66$ nm, and $tB_3 = 81.31$ nm. The number of layers per stack is 80. The corresponding value of ϕ is 1.639. The GA parameters are as follows: population size of solutions = 500, number of generations = 100, tournament size = 5, $p_t = 0.8$, $p_c = 0.8$, and $p_m = 0.01$.

14.2.3 Application in LCD devices

Figure 14.13 is a proposed configuration of an LCD device that employs the WSPR film described here. The diagram illustrates how the WSPR film can enhance color saturation of the display. Only the optical components most relevant to the workings of the LCD unit are included in the schematic, including an edge-lit-type display. A light guide plate (LGP) is illuminated with the help of a light source placed to the side of the LGP. The wavelength

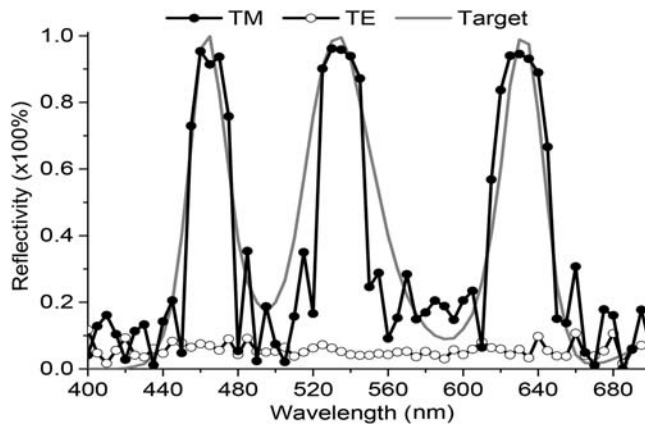


Figure 14.12 Reflectivity spectra of the WSPR film obtained after optimization.

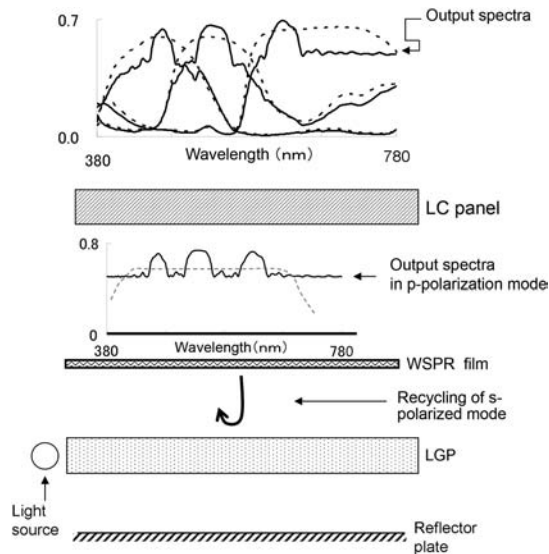


Figure 14.13 Illustration of the color-enhancing effect of the WSPR film when used in an LCD device.

spectrum of light transmitted from the WSPR film is shown. Light transmitted from the multilayer film is polarized primarily in the TE mode and is composed of the light that exits the light source and is transmitted directly through the multilayer film as well as the recycled light that returns after reflection. The light reflected from the multilayer film is polarized primarily in the TM mode and shows three peaks in the red, green, and blue regions of the visible spectrum. The amount and polarization state of the recycled light depend on the reflection spectrum of the reflector film at the back of the LGP and also depends on the existence of any diffuser plates or polarization converters that might be used in the path of light.

The light output at the multilayer film is computed as the sum of the directly transmitted light and the recycled light. We assume that 25% of the output is due to recycling. The wavelength spectrum of the output from the multilayer film is shown as a solid line in Fig. 14.13. For comparison purposes, the spectrum of output obtained with a conventional broadband multilayer film is also shown (as a dashed line). Clearly, the use of the wavelength-selective multilayer film leads to an output spectrum that depends strongly on the color of light.

The output from the multilayer film passes through the liquid crystal panel before it finally leaves the LCD device and reaches the observer. The liquid crystal (LC) panel consists of (at least) a conventional color filter and liquid crystal cells. The color filter is composed of at least three filters—red, green and blue—capable of transmitting the red, green, and blue portions of the visible light, respectively. Hence, the wavelength spectrum of the light emerging from

the LC panel is determined by the transmission properties of the color filter. The wavelength spectrum of the light exiting the LC panel is shown in Fig. 14.13. The solid line shows the output spectrum obtained with the WSPR film. The curve represented by the dashed line is obtained when a conventional, broadband multilayer film is used. A comparison between the two spectra shows that the WSPR film is more effective at cutting the light of unwanted wavelengths and improving the color saturation of the overall display device. Thus, from the point of view of improving color saturation, the WSPR film is clearly more desirable compared to the conventional, broadband multilayer film. The improvement in color saturation depends on the volume of the recycled light. The color saturation of the display device increases as the proportion of recycled light increases.

The color-enhancing capabilities of the WSPR film are not limited to those demonstrated in the LCD device model shown in Fig. 14.13. A real-life LCD device includes additional components, such as diffuser plates, $\lambda/4$ plates, etc. Similarly, an actual LC panel incorporates many other components such as polarizers, compensators, etc. Even with the addition of these extra components, the WSPR film would still remain useful in enhancing color saturation.

14.2.4 Discussion

This design method is not limited to $\lambda/4$ layers, meaning that solutions can be obtained for many different shapes (different bandwidths corresponding to three peaks) of the target spectrum. In the design process described here, Δn (the difference between refractive indices of the two layers along the x axis) and N (the total number of layers comprising the multilayer) are much smaller than those employed in multilayer polarizing films developed for broadband display application. The relatively smaller values for both Δn and N make such films easier and less expensive to fabricate. We found that the wavelength spectrum of the reflectivity of the multilayer depends strongly on the value of Δn . A desirable range for Δn is $0.02 < \Delta n < 0.25$. If Δn is greater than 0.25, reflectivity becomes high and uniform for a relatively broader band of wavelengths around the chosen peaks in the red, green, and blue regions of the visible spectrum. If $\Delta n < 0.02$, reflectivity peaks become unacceptably low.

Furthermore, the wavelength-selective reflectivity of the multilayer film designed here makes the film suitable for use with red, green, and blue LED light sources. By choosing optically isotropic materials for the layers of the basic units of the multilayer, it is possible to obtain the same wavelength-selective reflectivity in both TE and TM modes.

14.3 Summary

In Section 14.1, we presented a two-phase design process for multilayer WGP that find application as low-reflection polarizers in projection-type LCD

applications. A multilayer WGP is formed by adding thin layers on top of the metal ridges of an ordinary WGP. The addition of extra layers can help to reduce the reflection from the ordinary WGP while preserving the polarization efficiency. The reduction in reflection from the multilayer WGP depends on the number and material of these additional layers. The first phase of the design process employs an approximate computation scheme based on EMT and a characteristic matrix method for multilayers of thin films. In this phase, each WGP layer is approximated as a layer of thin film with an effective refractive index. In the second and final phase of design, the polarization-dependent reflection and transmission spectra of the WGP are computed using a FDTD method incorporating the dielectric FDTD and MRC-FDTD in two dimensions. The goal of the design process is to identify suitable materials and thicknesses for the additional thin layers needed to appreciably lower the reflection. The design method is explained with the help of bilayer WGP.

In Section 14.2, the design method and design results are presented for multilayer WSPR films that might be useful for LCD applications. The design method combines a characteristic matrix method with a GA-based optimization method.

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Appendix A

Supplemental Topics

Many other researchers have contributed to the advancement of the NS-FDTD methodology for computational electromagnetics and photonics. These researchers have extended the methodology to other various applications that cannot be covered in this book. With their permission, we provide in this chapter brief summaries and abstracts of several papers. In addition to those given below, there are many others in the extant literature that are too numerous to list. We thank our colleagues and collaborators in the NS-FDTD community for their contributions.

1. K. Taguchi, T. Ohtani, T. Kashiwa, and Y. Kanai, "The nonstandard FDTD method using a complex formulation," *IEEE Transactions on Magnetism* **40**(2), 1448–1451 (2004).

Summary: NS-FDTD can be expanded from the real domain into the complex to handle lossy materials. It can be applied to absorbing materials, surface impedance boundary condition (SIBC) materials, and dispersive materials.

Abstract

In this paper, a complex nonstandard finite-difference time-domain (CNS-FDTD) method is proposed in order to simulate wave propagation in lossy media. To clarify the characteristics of the method, expressions for the numerical propagation constant and the stability condition are derived. It is found that the CNS-FDTD method is much more accurate and stable than the conventional finite-difference time-domain (FDTD) method. The method is applied to the analysis of a fin-type ferrite electromagnetic wave absorber with a periodic structure.

2. T. Ohtani, K. Taguchi, T. Kashiwa, Y. Kanai, and J. B. Cole, "Nonstandard FDTD method for wideband analysis," *IEEE Transactions on Antennas and Propagation* **57**(8), 2386–2396 (2009).

Summary: The NS-FDTD can be expanded from monochromatic to wideband to handle pulse wave response. It can be applied to frequency response analysis, electromagnetic inference (EMI), and electromagnetic compatibility (EMC).

Abstract

The nonstandard (NS) FDTD algorithm can compute electromagnetic propagation with very high accuracy on a coarse grid, but only for monochromatic or narrow-band signals. We have developed a wideband (W) NS-FDTD algorithm that overcomes this limitation. In NS-FDTD special finite difference operators are used to make the numerical dispersion isotropic, which is then corrected by a frequency-dependent factor. In WNS-FDTD the numerical dispersion is modeled as frequency dependent electrical permittivity and magnetic permeability, and the Yee algorithm is augmented by correction terms in the time domain. We demonstrate the high accuracy of WNS-FDTD in example problems, and show that it gives better results than both the standard (S) FDTD and the FDTD(2,4) algorithms.

3. T. Ohtani and Y. Kanai, "Coefficients of finite difference operator for rectangular cell NS-FDTD method," *IEEE Transactions on Antennas and Propagation* **59**(1), 206–213 (2011).

Summary: The NS-FDTD can be expanded to handle noncubic hexagonals and can be applied to noncubic cells. A method to determine α for hexagonals is demonstrated.

Abstract

The nonstandard finite difference time domain (NS-FDTD) method is a dispersion error reduction technique for the FDTD method. High accuracy is achieved by the optimal selection of the coefficients used for the finite difference (FD) operators in the NS-FDTD method. However, the previously published method of obtaining the coefficients for rectangular cells, using a full numerical technique, takes an enormous amount of computing time. To solve this difficulty, we propose a semi-analytical method to obtain the optimal coefficients with a far higher computational efficiency. It is shown, by numerical tests, that the optimal coefficients need six significant digits for accurate NS-FDTD solutions. Consequently our new method can reduce the

computing time to obtain the optimal coefficients from an estimated 42×10^4 minutes by the previous method to about 7 seconds for three-dimensional rectangular cells.

4. T. Ohtani and Y. Kanai, "Optimal coefficients of the spatial finite difference operator for the complex nonstandard finite difference time-domain method," *IEEE Transactions on Magnetism* **47**(5), 1498–1501 (2011).

Summary: A method for determining operator weight coefficients for complex NS-FDTD is demonstrated.

Abstract

Optimal coefficients of the spatial finite difference (FD) operator for the complex nonstandard finite difference time-domain (CNS-FDTD) method are presented. To derive the optimal coefficients that minimize the dispersion error, we employ a semi-analytical method based on the FD Laplacian. The propagation constant is a complex number in lossy media; therefore, the derivation of the coefficients is more complicated than the derivation for the NS-FDTD method. It is confirmed by numerical tests using the numerical dispersion equation that our coefficients give the CNS-FDTD method a higher accuracy than the standard FDTD method. The coefficients are used for the reflection analysis of a grid ferrite electromagnetic wave absorber, and the validity of the coefficients is shown. The calculation time to derive the coefficients is negligible compared with that for the CNS-FDTD calculations themselves.

5. T. Ohtani, Y. Kanai, and N. V. Kantartzis, "A 4-D subgrid for the NS-FDTD technique using the CNS-FDTD algorithm with the Shepard method and a Gaussian smoothing filter," *IEEE Transactions on Magnetism* **51**(3), 7201004 (2015).

Summary: A subgrid technique using NS-FDTD to reduce computer resources is presented. The technique can be applied to the object, including a locally small geometry.

Abstract

A precise subgrid technique for the nonstandard finite-difference time-domain (NS-FDTD) method in 4-D (i.e., 3-D space and 1-D time) is proposed in this paper. The novel algorithm is efficiently blended with the Shepard scheme and a Gaussian smoothing filter to minimize the error in the interpolated values used for the spatial connection process. Moreover, the required

time interpolation is performed via the complex (C)NS-FDTD approach. A key advantage of the proposed formulation is its structural simplicity, due to the prior interpolation concepts and the absence of any nonphysical convention, which enables its straightforward application to a variety of realistic problems. The numerical results validate the benefits of the method by means of different subgrid simulation scenarios.

Appendix B

List of Programs and Instructions

B.1 Instructions for Mathcad Programs

The programs on the accompanying CD are written in Mathcad 15. To run them you need Mathcad installed on your computer. Without Mathcad you can see the source code and example outputs in the Program_Images file. In all Mathcad programs, we use the following settings and conventions.

Display Settings:

- (i) Windows Classic (necessary for some Mathcad graphics)
- (ii) Run program MCL.5_Color Maps to install customized color maps
- (iii) On some computers, the program regions may overlap. Use the “separate regions” command to correct this.

Worksheet Settings:

Automatic calculation is turned off.

Unit System: **none**

$\text{PRNPRECISION} = 8, \text{PRNCOLWIDTH} = 16$

Conventions:

$x := 10$, parameter x is defined to be 10. We advise that you not change it.

Yellow highlight, $x := 10$, indicates an example value of a parameter; change it if you like.

Green highlight, $x := 10$, indicates a recommended value of a parameter; be careful if you change it.

$x = 10$, echoes the value of computed or defined parameter.

Red highlight, $\Psi := \text{FDTD}(\Psi)$ click on this equation, and press F9.

disabled operation**enabled operation**FDTD := program1[■]

FDTD := program2.

[■]indicates that an operation is disabled (turned off).

In the above example, Program FDTD is defined to be program2. You can choose program1 instead by enabling the first definition and disabling the second.

B.2 List of Mathcad Programs

Chapter 2

MC2.1_DecayEquation

Finite difference solutions of the decay equation. Compares several different algorithms.

MC2.2_Relaxation

Relaxation algorithms to solve the 1D Poisson equation. Compares several different algorithms.

Chapter 5

MC5.1_AbsWaveEqn_Source

FDTD algorithms to solve the absorbing wave equation with a source. Compares several different algorithms.

MC5.2_TimeRevFDTD

Simple program to demonstrate time-reversed FDTD.

Chapter 6

MC6.1_ComputationalBoundaries

Demonstrates different computational boundary conditions.

MC6.2_NS_Amplitude

Nonstandard algorithm to extract wave amplitude in a real-number FDTD calculation in the presence of noise using three time samples.

MC6.3_NS_Spectrum

NS-FDTD calculation of transmission through a layer and comparison with the analytical result.

Chapter 7

MC7.1_FDTD_PtSource_vs_Analytic

Computes the field due to a point source using S- and NS-FDTD, and compares this with the analytic solution. S- and NS-Mur ABCs are implemented.

MC7.2_FDTD_ScattField

The S- and NS-FDTD scattered-field methodologies are used to compute scattering off of an infinite cylinder in the Mie regime, TE mode. Computations are compared with the analytic solution given by Mie theory. (Needs inputs from Program MC10.2.)

Chapter 9

MC9.1_S-Yee_1D

Simple program to demonstrate the standard Yee algorithm with the Mur ABC; choice of initial fields.

MC9.2_AltYee_1D

Alternative version of program MCP.9.1. Different layout of the electric and magnetic fields.

MC9.3_Yee_CurrSource_1D

One dimensional S- and NS-Yee algorithm with a current source; S- and NS-Mur ABC. Comparison with analytical solutions.

Chapter 10

MC10.1_TM_Yee_CurrSource

Implementation of the Yee algorithm with a current source in a homogeneous medium in the TM mode ($H_x = H_y = E_z = 0$); implementation of the Mur absorbing boundary and time reversal.

MC10.2_MieTheory_TE

The scattered field due to an infinite plane wave impinging on an infinite dielectric cylinder is computed using Mie theory in the TE mode ($E_x = E_y = H_z = 0$). (Inputs for Program MC7.2.)

MC10.3_TM_Yee_Scatterer

Current source generates an electromagnetic field that scatters off a dielectric object, TM mode ($H_x = H_y = E_z = 0$).

MC10.4_TM_Yee_Scatt_Fld

The S- and NS-Yee scattered field methodology is used to compute scattering off an infinite cylinder in the Mie regime, TM mode ($E_x = E_y = H_z = 0$). Computations are compared with the analytic solution given by Mie theory. (Needs inputs from Program MC10.5.)

MC10.5_MieTheory_TM

The scattered field due to an infinite plane wave impinging on an infinite dielectric cylinder is computed using Mie theory in the TM mode ($E_x = E_y = H_z = 0$). (Inputs for Program MC10.4.)

Chapter 12**MC12.1, RC-FDTD**

Recursion convolution FDTD for dispersive materials.

Chapter 13**MC13.1, Extinction Coefficients**

Computes the extinction coefficients in an RC-FDTD calculation.

MC13.2, Ellipsoid Spectra

Computes the extinction spectra of small ellipsoids.

Mathcad Program Library

Subroutines for the Mathcad programs listed above.

MCL.1_TE_Shapes

Produces simple geometric shapes using the staircase and fuzzy methodologies for use in the TE mode.

MCL.2_TM_Shapes

Produces simple geometric shapes using the staircase and fuzzy methodologies for use in the TM mode.

MCL.3_Visualization

Functions used to visualize field and intensity data.

MCL.4_2D_Interpolation

Interpolates data between grid points.

MCL.5_Color Maps

Creates additional color maps for data visualization.

B.3 Pseudocode Programs

Chapter 2

PC2.1, Parallel Relaxation in Serial Pseudocode

Parallel relaxation algorithm to solve the Poisson equation in one dimension, using a serial code.

PC2.2, Parallel Relaxation in Parallel Pseudocode

Parallel relaxation algorithm to solve the Poisson equation in one dimension, using a parallel code.

PC2.3, Forward Serial Relaxation Program in Serial Pseudocode

Solves the 1D Poisson equation.

PC2.4, Serial Over-Relaxation Program in Serial Pseudocode

Solves the 1D Poisson equation.

Chapter 9

PC9.1, Yee Algorithm in One Dimension

The 1D Yee algorithm, perfect Mur ABC.



James B. Cole and Saswatee Bannerjee,

*Computing the Flow of Light: Nonstandard FDTD
for Photonics Design*

SPIE Press, Bellingham, Washington (2017).

The supplemental files for this eBook are under SPIE copyright
and are available for download by copying and pasting the
following link to a browser:

http://spie.org/Samples/Pressbook_Supplemental/PM272_sup.zip

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