Chapter 3

Finite Difference Methods

The finite difference (FD) method transforms a differential equation or PDE into a difference equation that can be solved numerically. The basic elements of FD are as follows:

1. **Grid.** This is a set of points at which the unknown function in the PDE is sampled. Commonly, a grid is evenly spaced, so that in 1D the grid points can be written in the form $x_n = n\Delta x$, where $n = 1, 2, \ldots, N$. In 2D, a rectangular grid of points is often used, such that $(x_m, y_n) = (m\Delta x, n\Delta y)$. A rectangular or cubic 3D grid is defined similarly. Other types of grids include polar, hexagonal, and conformal. Conformal grids are used when it is advantageous to have grid points conform to the shape of a material object. For problems involving both space and time coordinates, a temporal grid for the time coordinate is also required.

2. **Stencil**. This is a difference approximation for the derivative of a quantity at one grid point in terms of values at neighboring points. The most common stencil for 1D problems is the first order central difference

$$\frac{\partial u(x)}{\partial y} \simeq \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x} \tag{3.1}$$

   Using a grid, this can be expressed as the difference equation $f(x_n) = [u(x_{n+1}) - u(x_{n-1})]/\Delta x$.

3. **Boundary Conditions**. At the edges of the grid, the stencil applied at points in the interior of the grid typically cannot be used. Some type of rule for handling the edge points is required. There are several different types of boundary conditions:

   - Dirichlet: $u|_{bd} = 0$. Sometimes instead of vanishing, the unknown may be equal to some given function at the boundary.
   - Neumann: $\frac{\partial u}{\partial n}\big|_{bd} = 0$, where n represents the coordinate that is normal to the boundary. Implementing this boundary condition on the FD grid using a forward difference approximation for the derivative leads to the relationship $x_1 = x_2$, where x_1 is a point on the grid boundary.
   - Mixed: A linear combination of f and its normal derivative are set to a constant.
   - Absorbing boundary condition (ABC): This type of boundary condition is very important in applications of the finite difference method. Most electromagnetics problems involve unbounded regions, which cannot be modeled computationally. One option is to use one of the above boundary conditions and make the simulation region very large, and terminate the simulation

before reflections from the boundary perturb the solution in the region of interest. The drawback of this approach is that the larger the simulation region, the greater the computational cost of the simulation. A better approach is to use a boundary condition that absorbs waves and reflects as little energy as possible. This is the computational analogue of an anechoic chamber. There are several types of ABCs, including:

One-way wave equation. These are easy to implement but imperfect in 2D and higher dimensions.

Perfectly matched layer with loss.

Surface integral equation on the boundary (MOM-TDIE).

Boundary conditions may also be required at material interfaces inside the simulation region.

4. **Solution method**. Applying a stencil at each grid points leads to a system of difference equations which can be solved for the unknown sample values. Solution methods can be grouped into two categories:

   - Explicit: update the value at one grid point at a time in terms of neighboring values.
   - Implicit: Arrange the difference equations into a linear system and solve for all of the unknowns at one time.

3.1 Hyperbolic PDEs - FDTD-1D

The simplest hyperbolic PDE is the 1D wave equation

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2 u(x,t)}{\partial t^2} \tag{3.2}$$

One physical problem that is modeled by this PDE is a planar time-domain current source that varies in intensity only in the x direction. Since the source varies only in the x direction, the radiated electric field also only varies in the x direction, and the components $E_y(x,t)$ and $E_z(x,t)$ both satisfy Eq. (3.2) where the source is zero.

In order to apply the finite difference method to the wave equation, difference approximations for the derivatives are required. The stencil for the second derivative in x is

$$\begin{aligned} \frac{\partial^2 u(x)}{\partial x^2} &\simeq \frac{\partial}{\partial x}\left[\frac{u(x+\Delta x/2)-u(x-\Delta x/2)}{\Delta x}\right] \\ &\simeq \frac{u(x+\Delta x)-2u(x)+u(x-\Delta x)}{(\Delta x)^2} \end{aligned} \tag{3.3}$$

where the t dependence of $u(x,t)$ is suppressed for brevity. The stencil for the right-hand side of (3.2) is very similar. Substituting difference approximations into the wave equation leads to

$$r^2\left[u(x+\Delta x,t)-2u(x,t)+u(x-\Delta x,t)\right] = u(x,t+\Delta t)-2u(x,t)+u(x,t-\Delta t) \tag{3.4}$$

where $r = c\Delta t/\Delta x$.

If we define a grid by the points $x_n = (n-1)\Delta x$ and $t_n = (n-1)\Delta t$, then $u(x_m,t_n) = u[(m-1)\Delta x,(n-1)\Delta t]$. As a shorthand notation, we write this as u_m^n. The difference equation becomes

$$r^2\left(u_{m+1}^n - 2u_m^n + u_{m-1}^n\right) = u_m^{n+1} - 2u_m^n + u_m^{n-1} \tag{3.5}$$

Now, we can solve this for u^{n+1} to obtain an explicit finite difference method:

$$u_m^{n+1} = r^2 \left(u_{m+1}^n - 2u_m^n + u_{m-1}^n\right) + 2u_m^n - u_m^{n-1} \tag{3.6}$$

This algorithm is known as the finite difference time domain method (FDTD), because a time coordinate is involved.

Initial Condition

Because the wave equation involves time, part of the boundary condition required for the finite difference approach is actually a boundary condition in time, or an initial condition. Since the PDE involves a second order time derivative, initial conditions at two time steps are required. This means that u_m^1 and u_m^2 must be specified as given functions. One common situation is the initial condition $u_m^1 = u_m^2 = 0$, and a source is applied at one of the spatial boundaries of the region.

Boundary Conditions

The simplest boundary condition is Dirichlet: $u(0,t) = 0$ and $u(d,t) = 0$, where $[0,d]$ is the simulation region. The Neumann condition is implemented by setting the endpoint value equal to the point next to it: $u_2^n = u_1^n$, and similarly for the right boundary point.

An absorbing boundary condition can be obtained by discretizing the one-way wave equation at the end-points of the region. This is known as the Mur boundary condition. At the right-hand side, we enforce the PDE

$$\frac{\partial u}{\partial x} = -\frac{1}{c}\frac{\partial u}{\partial t} \tag{3.7}$$

This equation has solutions of the form $u(x,t) = u_0(x - ct)$, which is a wave of arbitrary shape moving to the right as time increases. This allows waves to move out of the simulation region without reflection. We have to be careful in discretizing this equation, because the approximations for the spatial and time derivatives in the one-way wave equation need to be evaluated at the same point. This can be accomplished using averaging of sample values of u:

$$\frac{1}{2}\left(\underbrace{\frac{u_N^m - u_{N-1}^m}{\Delta x}}_{\text{at } (x_N - \Delta x/2, t_m)} + \underbrace{\frac{u_N^{m+1} - u_{N-1}^{m+1}}{\Delta x}}_{\text{at } (x_N - \Delta x/2, t_{m+1})}\right) = -\frac{1}{2c}\left(\underbrace{\frac{u_N^{m+1} - u_N^m}{\Delta t}}_{\text{at } (x_N, t_m + \Delta t/2)} + \underbrace{\frac{u_{N-1}^{m+1} - u_{N-1}^m}{\Delta t}}_{\text{at } (x_{N-1}, t_m + \Delta t/2)}\right) \tag{3.8}$$

By averaging the derivatives at two different locations, both derivative approximations in this expression are evaluated at the point $(x_N - \Delta x/2, t_m + \Delta t/2)$. Solving for u_N^{m+1} gives

$$u_N^{m+1} = u_{N-1}^m + \frac{r-1}{r+1}(u_{N-1}^{m+1} - u_N^m) \tag{3.9}$$

The boundary condition at $x = 0$ can be derived similarly. For 1D problems, the Mur ABC is a perfect absorber.

Sources

There are two types of sources that can be used in the FDTD method, hard sources and soft sources. A hard source simply sets the value of the field at one or more grid points equal to a specified function of time, and so is a type of Dirichlet boundary condition. This corresponds to an EM problem in which the electric field at some point is known, and we wish to find the values of the radiated field at other points. One property of a hard source is that waves propagating towards the source are reflected by the source.

A soft source corresponds to an impressed electric current. In order to allow for a soft source, we must rederive (3.2) from Maxwell's equations. If we take the curl of Faraday's law and substitute in Ampere's law, we obtain

$$\nabla \times \nabla \times \overline{\mathcal{E}} + \frac{1}{c^2}\frac{\partial^2 \overline{\mathcal{E}}}{\partial t^2} = -\mu \frac{\partial \overline{\mathcal{J}}}{\partial t} \tag{3.10}$$

where $c = 1/\sqrt{\mu\epsilon}$. If we use the vector calculus identity

$$-\nabla \times \nabla \times \overline{\mathcal{E}} + \nabla(\nabla \cdot \overline{\mathcal{E}}) = \nabla^2 \overline{\mathcal{E}} \tag{3.11}$$

and assume that the permittivity is constant and the net electric charge is zero, so that $\nabla \cdot \overline{\mathcal{D}} = \nabla \cdot \overline{\mathcal{E}} = 0$, then we arrive at the wave equation

$$\nabla^2 \overline{\mathcal{E}} - \frac{1}{c^2}\frac{\partial^2 \overline{\mathcal{E}}}{\partial t^2} = \mu \frac{\partial \overline{\mathcal{J}}}{\partial t} \tag{3.12}$$

For a problem in which the current density vector is in one direction only, and the source varies also only in one direction, this reduces to a 1D wave equation of the same form as (3.2) but with a forcing function determined by the current source. If Eq. (3.12) is discretized using the finite difference method, we arrive at the difference equation

$$u_m^{n+1} = r^2\left(u_{m+1}^n - 2u_m^n + u_{m-1}^n\right) + 2u_m^n - u_m^{n-1} - c^2(\Delta t)^2 \mu \left.\frac{\partial J(x_m,t)}{\partial t}\right|_{t=t_n} \tag{3.13}$$

where u represents a component of the electric field. A time harmonic plane current of the form $J_y = J_0 \sin(\omega t)\delta(x - x_s)$ launches plane waves traveling away from the source on both sides. To obtain a plane wave with an electric field of amplitude E_0, using the fact that the discretized source has a width Δx, the difference equation becomes

$$u_m^{n+1} = r^2\left(u_{m+1}^n - 2u_m^n + u_{m-1}^n\right) + 2u_m^n - u_m^{n-1} - 2r\omega\Delta t E_0 \cos(\omega t_n)\delta_{m,m_s} \tag{3.14}$$

where $x_{m_s} = x_s$ is the location of the source.

One problem with a soft source is that in general it leads to a nonzero DC component in the solution. To avoid this, the modified source function [Cyntha Furse, *et al.*, IEEE Transactions on Antennas and Propagation, vol. 48, Aug. 2000, pp. 1198-1201]

$$r(t)\sin(\omega t) \tag{3.15}$$

can be used. The function $r(t)$ is a turn-on function defined by

$$r(t) = \begin{cases} 0 & t < 0 \\ 0.5[1 - \cos(\omega t/(2\alpha))] & 0 \le t \le \alpha T \\ 1 & t > \alpha T \end{cases} \tag{3.16}$$

where T is the period of the time-harmonic source and $\alpha = 1/2, 3/2, 5/2, \ldots$.

3.1.1 Stability

By running simulations for different values of Δx and Δt, it is easy to see that the FDTD method is unstable for some values of the discretization lengths. We can study the solution to the FDTD difference equation analytically to gain insight into this problem. A single-frequency solution to the 1D wave equation is

$$u(x,t) = \cos(kx \pm \omega t) \tag{3.17}$$

where $k = \omega/c$. For convenience in the following analysis, we use the fact that $\sin(kx \pm \omega t)$ is also a solution to put this into complex exponential form $e^{jkx+j\omega t}$. The FDTD-1D difference equation has a discrete solution of similar form:

$$u_m^n = e^{jkm\Delta x + j\omega n\Delta t} \tag{3.18}$$

By substituting this solution into the difference equation, we can obtain a dispersion relation that will be different from the free space dispersion relation $k = \omega/c$.

This procedure leads to the relationship

$$\cos(\omega\Delta t) = r^2[\cos(k\Delta x) - 1] + 1 \tag{3.19}$$

This is the numerical dispersion relation for the FDTD-1D algorithm. Notice that if the right-hand side of (3.19) is greater than one in magnitude for some value of k, then ω must have a nonzero imaginary part. If this is the case, then the time exponential in solution (3.18) becomes a real exponential, and the solution blows up as time increases. Restricting the right-hand side of (3.19) to be less than or equal to one in magnitude leads to the stability criterion

$$\frac{c\Delta t}{\Delta x} \leq 1 \tag{3.20}$$

This condition leads to a nice physical picture. If we consider a given grid point (x_m, t_n), the light cone for that point is defined to be all points in the future that can be reached by traveling at the speed of light. If (3.20) is met, then only one grid point at the $n + 1$ time step is inside the light cone. If more than one grid point at the next time step were inside the cone, then in a loose sense, too much energy is transferred from the solution at one time step to the solution at the next time step, and unwanted signal amplification occurs.