I The FDTD (Finite Difference Time Domain) Algorithm

The FDTD method refers to a specific FD discretization of the time dependent Maxwell's equations. It has been developed by Yee in 1966. It is based on a Cartesian grid.

I.1 Maxwell's Equations

In a source free (no electric or magnetic sources) region of space, Maxwell's equations are

$$\begin{aligned}
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}, \quad \text{(Faraday's law)} \\
\nabla \times \mathbf{H} &= \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_c, \quad \text{(Ampere's law)} \\
\nabla \cdot \mathbf{D} &= 0, \\
\nabla \cdot \mathbf{B} &= 0.
\end{aligned}$$

In a linear, isotropic, non-dispersive material (i.e. materials having field independent, direction independent, and frequency independent electric and magnetic properties)

$$\mathbf{D} = \varepsilon \mathbf{E}, \quad \mathbf{B} = \mu \mathbf{H}, \quad \mathbf{J}_c = \sigma \mathbf{E}$$

where ε, μ, and σ are called the constitutive parameters, we can write

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \mathbf{E}, \tag{1}$$

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \mathbf{H} - \frac{\sigma}{\varepsilon} \mathbf{E}. \tag{2}$$

In Cartesian coordinates we have

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y}\right) \tag{1a}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z}\right) \tag{1b}$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}\right) \tag{1c}$$

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x\right) \tag{2a}$$

$$\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y\right) \tag{2b}$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_{yz}\right) \tag{2c}$$

which form a system of 6 coupled PDE's in the 6 field components.

Notation: We have 4 independent variables, x, y, z, and t. We will consider discretization in each of these variables. Let $u\left(x, y, z, t\right)$ denote any of the 6 field components. We will denote a grid point in space by

$$(i\Delta x, j\Delta y, k\Delta z) = (i, j, k)$$

and a time instant by

$$t = n\Delta t$$

where i, j, k, and n are integers. Then

$$u\left(i\Delta x, j\Delta y, k\Delta z, n\Delta t\right) = u^n\left(i, j, k\right).$$

I.2 The Yee Algorithm

Yee used central difference expressions to approximate the derivatives. Consider (1a)

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu}\left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y}\right) \tag{1a}$$

At time step n we can write a central difference to the LHS as

$$\frac{H_x^{n+\frac{1}{2}}(i,j,k) - H_x^{n-\frac{1}{2}}(i,j,k)}{\Delta t}.$$

Thus

$$\frac{H_x^{n+\frac{1}{2}}(i,j,k) - H_x^{n-\frac{1}{2}}(i,j,k)}{\Delta t} =$$

$$\frac{1}{\mu(i,j,k)}\left[\frac{E_y^n\left(i,j,k+\frac{1}{2}\right) - E_y^n\left(i,j,k-\frac{1}{2}\right)}{\Delta z}\right.$$

$$\left. - \frac{E_z^n\left(i,j+\frac{1}{2},k\right) - E_z^n\left(i,j-\frac{1}{2},k\right)}{\Delta y}\right] \tag{1a$'$}$$

Here $\mu(i,j,k)$ denotes the permeability at a space point, and this takes inhomogeneous media into account.

Note: We are assuming that the corresponding cell is homogeneous. We will consider the more general case later.

The Yee algorithm is a "marching on in time" algorithm. That is, we assume that all field values are given at initial time $t = 0$, or equivalently for $n = 0$. Then we proceed to calculate field values at $\Delta t/2, \quad \Delta t, \quad 3\Delta t/2, \quad 2\Delta t, \ldots$ i.e. for $n = 1/2, \quad 1, \quad 3/2, \quad 2, \ldots$.

Eq. (1a′) therefore defines $H_x(i,j,k)$ at time step $n+1/2$ in terms of previously calculated values of H_x (at time step $n-1/2$), E_y and E_z (at time step n). Thus we have

$$H_x^{n+\frac{1}{2}}(i,j,k) = H_x^{n-\frac{1}{2}}(i,j,k) + \frac{\Delta t}{\mu(i,j,k)}\left[\frac{E_y^n\left(i,j,k+\frac{1}{2}\right) - E_y^n\left(i,j,k-\frac{1}{2}\right)}{\Delta z} - \frac{E_z^n\left(i,j+\frac{1}{2},k\right) - E_z^n\left(i,j-\frac{1}{2},k\right)}{\Delta y}\right] \qquad (1a'')$$

Now consider (2a)

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x\right) \tag{2a}$$

If we use time step n as the center point, we would need H at n, i.e. at full-steps. However, (1a$''$) gives magnetic field values at half-steps. This can be avoided if we discretize (2a) at time step $n+1/2$. Thus

$$
\begin{aligned}
&\frac{E_x^{n+1}(i,j,k) - E_x^{n}(i,j,k)}{\Delta t} = \\
&\frac{1}{\varepsilon(i,j,k)} \frac{H_z^{n+\frac{1}{2}}\left(i, j+\frac{1}{2}, k\right) - H_z^{n+\frac{1}{2}}\left(i, j-\frac{1}{2}, k\right)}{\Delta y} \\
&- \frac{1}{\varepsilon(i,j,k)} \frac{H_y^{n+\frac{1}{2}}\left(i, j, k+\frac{1}{2}\right) - H_y^{n+\frac{1}{2}}\left(i, j, k-\frac{1}{2}\right)}{\Delta z} \\
&- \frac{\varepsilon(i,j,k)}{\sigma(i,j,k)} E_x^{n+\frac{1}{2}}(i,j,k) \qquad \text{(2a}'\text{)}
\end{aligned}
$$

Note that we still have E_x at time step $n + 1/2$. If we can find an approximation to $E_x^{n+\frac{1}{2}}(i, j, k)$ in terms of electric field values at full time steps, we could avoid the calculation of E field at half steps. For this purpose we write

$$E_x^{n+\frac{1}{2}}(i, j, k) \simeq \frac{E_x^{n+1}(i, j, k) + E_x^{n}(i, j, k)}{2}.$$

Using this in (2a$'$) we can express $E_x^{n+1}(i, j, k)$ in terms of previously calculated values:

$$E_x^{n+1}(i,j,k) = \frac{1 - \frac{\sigma(i,j,k)\Delta t}{2\varepsilon(i,j,k)}}{1 + \frac{\Delta t \sigma(i,j,k)}{2\varepsilon(i,j,k)}} E_x^n(i,j,k)$$

$$+ \frac{\frac{\Delta t}{\varepsilon(i,j,k)}}{1 + \frac{\sigma(i,j,k)\Delta t}{2\varepsilon(i,j,k)}} \left[\frac{H_z^{n+\frac{1}{2}}\left(i, j+\frac{1}{2}, k\right) - H_z^{n+\frac{1}{2}}\left(i, j-\frac{1}{2}, k\right)}{\Delta y} \right.$$

$$\left. - \frac{H_y^{n+\frac{1}{2}}\left(i, j, k+\frac{1}{2}\right) - H_y^{n+\frac{1}{2}}\left(i, j, k-\frac{1}{2}\right)}{\Delta z} \right] \qquad (2\text{a}'')$$

Note that (2a$''$) expresses E_x at time step $n+1$ in terms of previously calculated values of E_x (at time step n), H_y and H_z (at time step $n+1/2$).

In a similar way the finite difference expressions for

$H_y^{n+\frac{1}{2}}(i,j,k)$ can be obtained from (1b),

$H_z^{n+\frac{1}{2}}(i,j,k)$ can be obtained from (1c),

$E_y^{n+1}(i,j,k)$ can be obtained from (2b),

$E_z^{n+1}(i,j,k)$ can be obtained from (2c).

The final equations are

$$H_x^{n+\frac{1}{2}}\left(i,j,k\right) = H_x^{n-\frac{1}{2}}\left(i,j,k\right)$$
$$+\frac{\Delta t}{\mu\left(i,j,k\right)}\left[\frac{E_y^n\left(i,j,k+\frac{1}{2}\right) - E_y^n\left(i,j,k-\frac{1}{2}\right)}{\Delta z} - \frac{E_z^n\left(i,j+\frac{1}{2},k\right) - E_z^n\left(i,j-\frac{1}{2},k\right)}{\Delta y}\right]$$

$$H_y^{n+\frac{1}{2}}\left(i,j,k\right) = H_y^{n-\frac{1}{2}}\left(i,j,k\right)$$
$$+\frac{\Delta t}{\mu\left(i,j,k\right)}\left[\frac{E_z^n\left(i+\frac{1}{2},j,k\right) - E_z^n\left(i-\frac{1}{2},j,k\right)}{\Delta x} - \frac{E_x^n\left(i,j,k+\frac{1}{2}\right) - E_x^n\left(i,j,k-\frac{1}{2}\right)}{\Delta z}\right]$$

$$H_z^{n+\frac{1}{2}}\left(i,j,k\right) = H_z^{n-\frac{1}{2}}\left(i,j,k\right)$$
$$+\frac{\Delta t}{\mu\left(i,j,k\right)}\left[\frac{E_x^n\left(i,j+\frac{1}{2},k\right) - E_x^n\left(i,j-\frac{1}{2},k\right)}{\Delta y} - \frac{E_y^n\left(i+\frac{1}{2},j,k\right) - E_y^n\left(i-\frac{1}{2},j,k\right)}{\Delta x}\right]$$

Define

$$C_{i,j,k} = \frac{1 - \frac{\sigma(i,j,k)\Delta t}{2\varepsilon(i,j,k)}}{1 + \frac{\Delta t \sigma(i,j,k)}{2\varepsilon(i,j,k)}}, \qquad D_{i,j,k} = \frac{\frac{\Delta t}{\varepsilon(i,j,k)}}{1 + \frac{\sigma(i,j,k)\Delta t}{2\varepsilon(i,j,k)}}$$

$$E_x^{n+1}(i,j,k) = C_{i,j,k} E_x^n(i,j,k)$$

$$+D_{i,j,k}\left[\frac{H_z^{n+\frac{1}{2}}\left(i,j+\frac{1}{2},k\right) - H_z^{n+\frac{1}{2}}\left(i,j-\frac{1}{2},k\right)}{\Delta y} - \frac{H_y^{n+\frac{1}{2}}\left(i,j,k+\frac{1}{2}\right) - H_y^{n+\frac{1}{2}}\left(i,j,k-\frac{1}{2}\right)}{\Delta z}\right]$$

$$E_y^{n+1}(i,j,k) = C_{i,j,k} E_y^n(i,j,k)$$

$$+D_{i,j,k}\left[\frac{H_x^{n+\frac{1}{2}}\left(i,j,k+\frac{1}{2}\right) - H_x^{n+\frac{1}{2}}\left(i,j,k-\frac{1}{2}\right)}{\Delta z} - \frac{H_z^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k\right) - H_z^{n+\frac{1}{2}}\left(i-\frac{1}{2},j,k\right)}{\Delta x}\right]$$

$$E_z^{n+1}(i,j,k) = C_{i,j,k} E_z^n(i,j,k)$$

$$+D_{i,j,k}\left[\frac{H_y^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k\right) - H_y^{n+\frac{1}{2}}\left(i-\frac{1}{2},j,k\right)}{\Delta x} - \frac{H_x^{n+\frac{1}{2}}\left(i,j+\frac{1}{2},k\right) - H_x^{n+\frac{1}{2}}\left(i,j-\frac{1}{2},k\right)}{\Delta y}\right]$$

These equations show that we need **E** at full time steps and **H** at half time steps as shown. Yee algorithm computes **E** and **H** field components at alternating time steps in a "leapfrog" arrangement.

E is calculated at time steps $t = 0, \Delta t, 2\Delta t, \ldots$

H is calculated at time steps $t = 0.5\Delta t, 1.5\Delta t, 2.5\Delta t, \ldots$

They are also displaced by half steps in space.

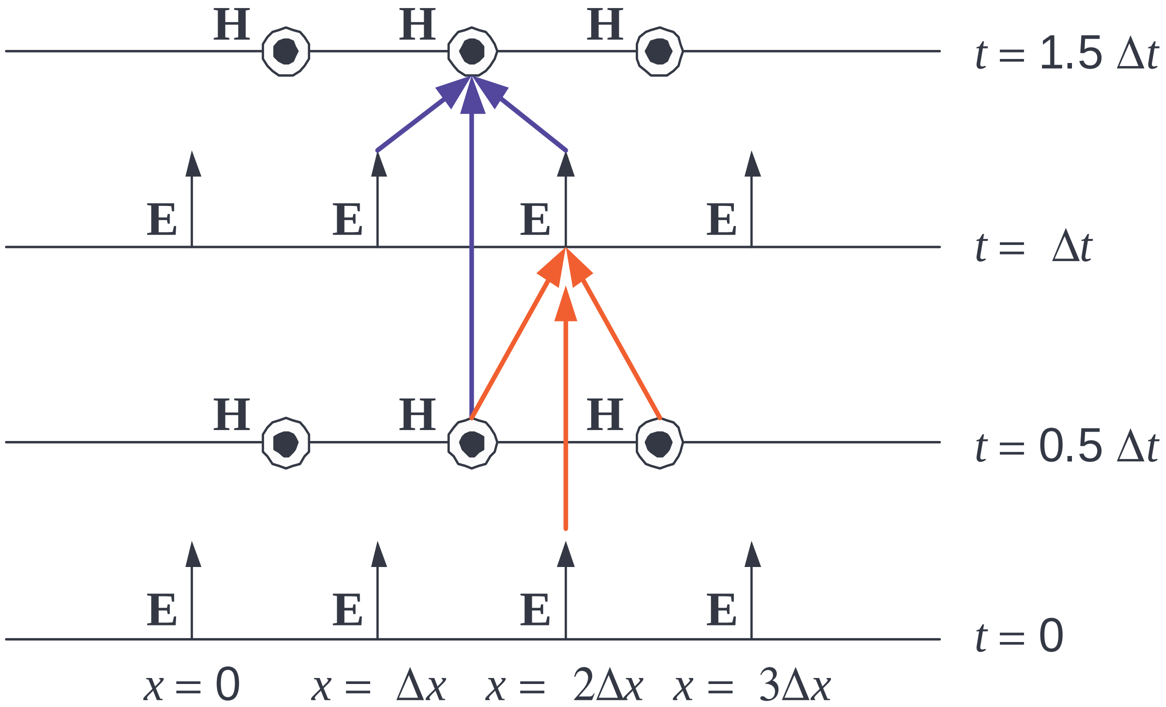

Figure.1: Space-time chart of the Yee algorithm for a 1-D wave propagation example showing the use of central differences for space derivatives and leapfrog for the time derivatives.

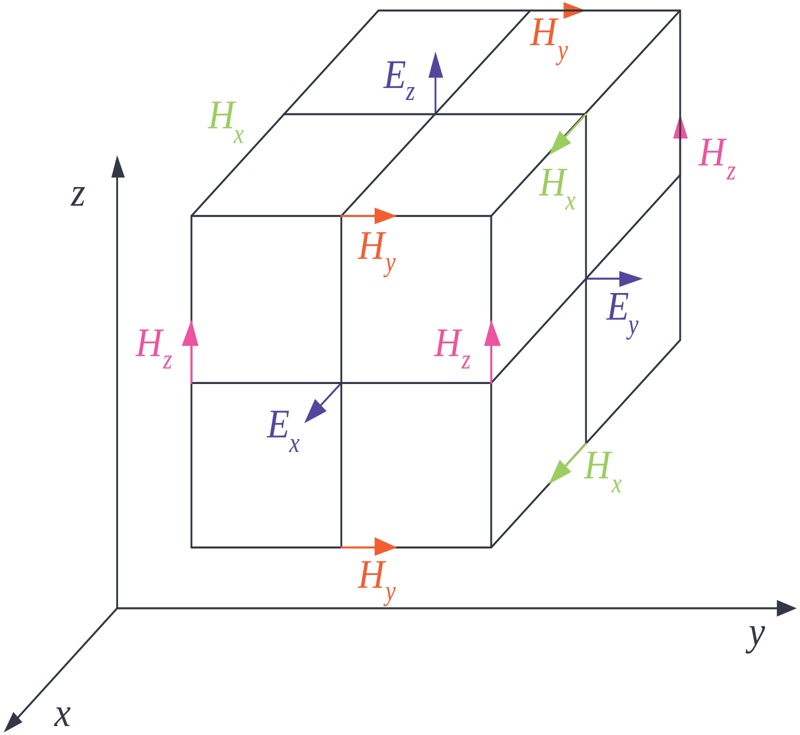

Figure.2: A cubic cell of Yee space lattice.

In the space coordinates we don't need to calculate the E and H field components at every point. Suppose that the coordinates of the center point of the Yee space lattice is (i, j, k). Then, we need to calculate

$$
\begin{aligned}
&E_x^n\left(i+\frac{1}{2}, j, k\right), \qquad H_x^{n+\frac{1}{2}}\left(i, j+\frac{1}{2}, k+\frac{1}{2}\right), \\
&E_y^n\left(i, j+\frac{1}{2}, k\right), \qquad H_y^{n+\frac{1}{2}}\left(i+\frac{1}{2}, j, k+\frac{1}{2}\right), \\
&E_y^n\left(i, j, k+\frac{1}{2}\right), \qquad H_z^{n+\frac{1}{2}}\left(i+\frac{1}{2}, j+\frac{1}{2}, k\right).
\end{aligned}
$$

In the Yee space lattice every $\mathbf{E}$ is surrounded by four circulating $\mathbf{H}$ components, and every $\mathbf{H}$ component is surrounded by four circulating $\mathbf{E}$ components.

Let the coordinates of the center point of the lattice cell be (i, j, k). Consider the front face. The coordinates of the center point of the front face is $\left(i+\frac{1}{2}, j, k\right)$. Then $E_x\left(i+\frac{1}{2}, j, k\right)$ is expressed in terms of H_z values at the left and at the right i.e. $H_z\left(i+\frac{1}{2}, j-\frac{1}{2}, k\right)$ and $H_z\left(i+\frac{1}{2}, j+\frac{1}{2}, k\right)$ and H_y values above and below, i.e. $H_y\left(i+\frac{1}{2}, j, k+\frac{1}{2}\right)$ and $H_y\left(i+\frac{1}{2}, j, k-\frac{1}{2}\right)$ (and also the value of E_x at (i, j, k)). This is the physical explanation of ($2a''$). Similarly, the right face corresponds to ($2b''$) and the top face to ($2c''$).

The Yee algorithm for FDTD was originally obtained by replacing the derivatives in the point form of Maxwell's curl equations by central difference formulas. However, the integral forms of Maxwell's equations can also be used to obtain the same formulas.

I.3 Integral Formulation

We start with Maxwell's curl equations again.

$$\nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E} \tag{1}$$

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} \tag{2}$$

We choose two surfaces S_E and S_H bounded by the curves C_E and C_H. Integrating (1) over S_E and using Stokes' theorem gives

$$\oint_{C_E} \mathbf{E} \cdot d\mathbf{l} = \int_{S_E} \mu \frac{\partial \mathbf{H}}{\partial t} \cdot \mathbf{n} dS. \tag{3}$$

Similarly, integrating (2) over S_H and using Stokes' theorem gives

$$\oint_{C_H} \mathbf{H} \cdot d\mathbf{l} = \int_{S_H} \varepsilon \frac{\partial \mathbf{E}}{\partial t} \cdot \mathbf{n} dS + \int_{S_H} \sigma \mathbf{E} \cdot \mathbf{n} dS. \qquad (4)$$

Eq.s (3) and (4) are the integral forms of the Maxwell's curl equations and are equivalent to the differential forms.

To simplify the derivation let us consider a linearly polarized TEM$_z$ electromagnetic wave propagating in the positive z direction.

We can write

$$\mathbf{E} = E_x(z,t)\,\mathbf{a}_x$$
$$\mathbf{H} = H_y(z,t)\,\mathbf{a}_y$$

In general, ε, μ, and σ are functions of position and for simplicity we will assume that they are functions of z only.

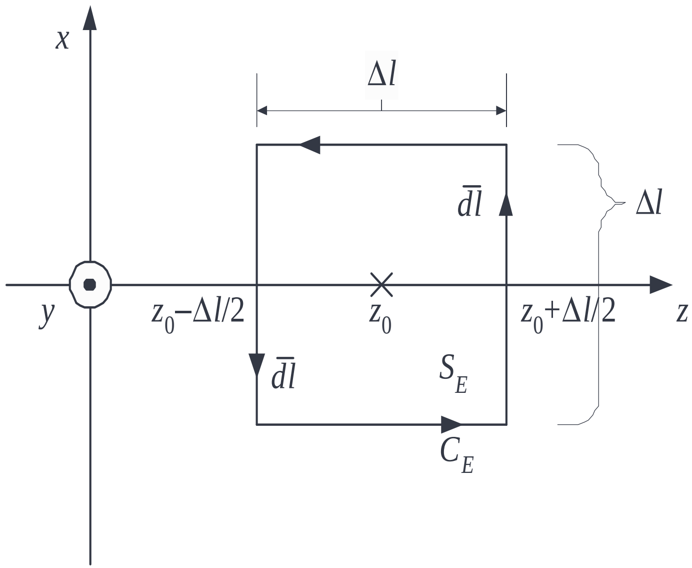

Figure.3: Contour for integration of (3).

With the choice of S_E shown in Fig. (3), we can approximate the LHS of (3) as:

$$\oint_{C_E} \mathbf{E}\cdot d\mathbf{l} = \underbrace{-E_x\left(z_0-\frac{\Delta l}{2},t\right)\Delta l}_{\substack{\text{on the left path}\\ d\mathbf{l}\text{ and }\mathbf{E}\text{ are in}\\ \text{opposite directions}}} + \underbrace{E_x\left(z_0+\frac{\Delta l}{2},t\right)\Delta l}_{\substack{\text{on the right path}\\ d\mathbf{l}\text{ and }\mathbf{E}\text{ are in}\\ \text{the same direction}}}$$

Note that on the top and bottom paths $d\mathbf{l}$ and $\mathbf{E}$ are orthogonal and line integrals are zero.

For the RHS of (3), we have

$$-\int_{S_E} \mu \frac{\partial \mathbf{H}}{\partial t} \cdot \underbrace{\mathbf{n}}_{\mathbf{a}_y} dS = -\int_{S_E} \mu \frac{\partial H_y(z,t)}{\partial t} \underbrace{dS}_{dzdx}$$

If Δl is *sufficiently small*, $\partial H_y(z,t)/\partial t$ can be taken as $\partial H_y(z_0,t)/\partial t$. Then the RHS becomes

$$\begin{aligned} -\int_{S_E} \mu \frac{\partial H_y(z,t)}{\partial t} dxdz &\simeq -\frac{\partial H_y(z_0,t)}{\partial t} \int_{S_E} \mu(z)\, dxdz \\ &= -\frac{\partial H_y(z_0,t)}{\partial t} \Delta l \int_{z_0-\frac{\Delta l}{2}}^{z_0+\frac{\Delta l}{2}} \mu(z)\, dz \end{aligned}$$

Note that the average value of μ (denoted μ_{avg}) is

$$\mu_{avg} = \frac{1}{\Delta l} \int_{z_0 - \frac{\Delta l}{2}}^{z_0 + \frac{\Delta l}{2}} \mu\left(z\right) dz$$

hence

$$-\int_{S_E} \mu \frac{\partial H_y\left(z, t\right)}{\partial t} dx dz = -\mu_{avg} \frac{\partial H_y\left(z_0, t\right)}{\partial t} \left(\Delta l\right)^2$$

Eq. (3) reduces to

$$\frac{E_x\left(z_0 + \frac{\Delta l}{2}, t\right) \Delta l - E_x\left(z_0 - \frac{\Delta l}{2}, t\right) \Delta l}{\Delta l} = -\mu_{avg} \frac{\partial H_y\left(z_0, t\right)}{\partial t}$$

Finally, using central difference approximation to the time derivative we get

$$\frac{E_x\left(z_0+\frac{\Delta l}{2},t\right)\Delta l - E_x\left(z_0-\frac{\Delta l}{2},t\right)\Delta l}{\Delta l} = \\ -\mu_{avg}\frac{H_y\left(z_0,t+\frac{\Delta t}{2}\right)-H_y\left(z_0,t-\frac{\Delta t}{2}\right)}{\Delta t}$$

The integral formulation shows that when the constitutive parameters vary within a Yee cell, their average values should be used. This becomes important especially at the interface of two media. The differential aprroach is straightforward but fails to give an answer to such cases.

Now consider the front surface of the Yee lattice shown in Fig. (2). Applying a similar derivation for (4) at time step $n+\frac{1}{2}$ we get

$$H_y^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k-\frac{1}{2}\right)\Delta y+H_z^{n+\frac{1}{2}}\left(i+\frac{1}{2},j+\frac{1}{2},k\right)\Delta z$$
$$-H_y^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k+\frac{1}{2}\right)\Delta y-H_z^{n+\frac{1}{2}}\left(i+\frac{1}{2},j-\frac{1}{2},k\right)\Delta z=$$
$$\varepsilon_{avg}\left(i+\frac{1}{2},j,k\right)\frac{E_x^{n+1}\left(i+\frac{1}{2},j,k\right)-E_x^{n}\left(i+\frac{1}{2},j,k\right)}{\Delta t}\Delta y\Delta z$$
$$+\sigma_{avg}\left(i+\frac{1}{2},j,k\right)\frac{E_x^{n}\left(i+\frac{1}{2},j,k\right)+E_x^{n+1}\left(i+\frac{1}{2},j,k\right)}{2}$$

where

$$E_x^{n+\frac{1}{2}}\left(i+\frac{1}{2},j,k\right)=\frac{E_x^n\left(i+\frac{1}{2},j,k\right)+E_x^{n+1}\left(i+\frac{1}{2},j,k\right)}{2}$$

which is similar to $(2a'')$ except for the fact that average values pf the constitutive parameters are used.

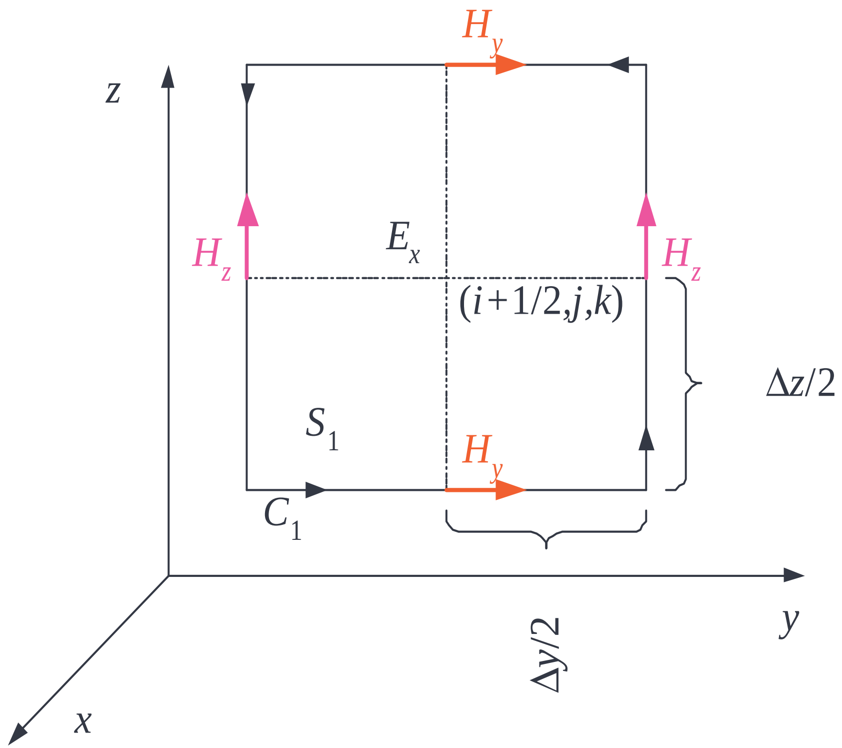

Figure.4: Contour for integration of (4).