Appendix 3 - Finite-Difference Power Relation and \( V^n \)

Consider Figure A3.1, three lump elements coincide with \( E_x(i,j,k) \), \( E_y(i,j,k) \) and \( E_z(i,j,k) \) in Cube (i,j,k). The current density for each element is \( J_x(i,j,k) \), \( J_y(i,j,k) \) and \( J_z(i,j,k) \).

![Figure A3.1 - Lump elements coincide with \( E_x(i,j,k) \), \( E_y(i,j,k) \) and \( E_z(i,j,k) \).](image)

The numerical power dissipation density \( (E \cdot J) \) at \( n + \frac{1}{2} \) time step for Cube (i,j,k) is taken as:

\[
P_{(i,j,k)}^{n+\frac{1}{2}} = \sum_{r=x,y,z} \frac{1}{2} \left( E_{r(i,j,k)}^{n+1} + E_{r(i,j,k)}^n \right) J_{r(i,j,k)}^{n+\frac{1}{2}} = (E \cdot J)_x^{n+\frac{1}{2}} + (E \cdot J)_y^{n+\frac{1}{2}} + (E \cdot J)_z^{n+\frac{1}{2}} \quad (A3.1)
\]

Consider the first term of (A3.1). Solving (6.2.1d) for \( J_{x(i,j,k)}^{n+\frac{1}{2}} \):

\[
(E \cdot J)_x^{n+\frac{1}{2}} = \frac{1}{2} \left( E_{x(i,j,k)}^{n+1} + E_{x(i,j,k)}^n \right) \left[ -\left( E_{x(i,j,k)}^{n+1} - E_{x(i,j,k)}^n \right) + \Delta t \frac{\Delta}{\varepsilon_{(i,j,k)}} \nabla \times H_{x(i,j,k)}^{n+\frac{1}{2}} \right] \left( \varepsilon_{x(i,j,k)} \Delta t \right)
\]

\[
= -\frac{1}{2} \left( \frac{\varepsilon_{x(i,j,k)}}{\Delta t} \right) \left[ \left( E_{x(i,j,k)}^{n+1} \right)^2 - \left( E_{x(i,j,k)}^n \right)^2 \right] + \frac{1}{2} \left( E_{x(i,j,k)}^{n+1} + E_{x(i,j,k)}^n \right) \left( \nabla \times H_{x(i,j,k)}^{n+\frac{1}{2}} \right)
\]

Now let us introduce three new notations:

\[
\left( E^n \cdot \nabla \times H_{x(i,j,k)}^{n+\frac{1}{2}} \right)_{(i,j,k)} = \sum_{r=x,y,z} E_{r(i,j,k)}^n \nabla \times H_{r(i,j,k)}^{n+\frac{1}{2}} \quad (A3.2)
\]

\[
\left( H_{r(i,j,k)}^{n+\frac{1}{2}} \cdot \nabla \times E^n \right)_{(i,j,k)} = \sum_{r=x,y,z} H_{r(i,j,k)}^{n+\frac{1}{2}} \nabla \times E_{r(i,j,k)}^n \quad (A3.3)
\]
\[ \nabla \left( E^{n+1} \times H^{n+\frac{1}{2}} \right)_{(i,j,k)} = -\left( E^{n+1} \cdot \nabla \times H^{n+\frac{1}{2}} \right)_{(i,j,k)} + \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} \]  

(A3.4)

In (A3.2)-(A3.4) the time-step is not critical, for instance we could replace \( n \) with \( n + 1 \) without affecting the validity. Using (A3.2) and summing up the x, y and z components, (A3.1) can be written in a more compact form:

\[ -P^{n+\frac{1}{2}}_{(i,j,k)} = \frac{1}{2} \left\{ \sum_{r=x,y,z} \frac{E_{(i,j,k)}}{\Delta t} \left( (E_{r(i,j,k)}^{n+1})^2 - (E_{r(i,j,k)}^n)^2 \right) - \left( E^{n+1} \cdot \nabla \times H^{n+\frac{1}{2}} \right)_{(i,j,k)} + \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} \right\} \]  

(A3.5)

Adding and subtracting \( \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} \) and \( \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^n \right)_{(i,j,k)} \) to the second and third terms on the right-hand side of (A3.5):

\[ \left( E^{n+1} \cdot \nabla \times H^{n+\frac{1}{2}} \right)_{(i,j,k)} \quad \text{and} \quad \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} \]  

(A3.6a)

\[ \left( E^n \cdot \nabla \times H^{n+\frac{1}{2}} \right)_{(i,j,k)} \quad \text{and} \quad \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^n \right)_{(i,j,k)} \]  

(A3.6b)

Using (A3.3), (6.2.1a)-(6.2.1c), the first term on the right-hand side of (A3.6a) and (A3.6b) can be expanded as:

\[ \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} = -\sum_{r=x,y,z} \frac{\mu}{\Delta t} \left\{ \left( H_{r(i,j,k)}^{n+\frac{1}{2}} \right)^2 - \left( H_{r(i,j,k)}^n \right)^2 \right\} + \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} \]  

(A3.7a)

\[ \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^n \right)_{(i,j,k)} = -\sum_{r=x,y,z} \frac{\mu}{\Delta t} \left\{ \left( H_{r(i,j,k)}^{n+\frac{1}{2}} \right)^2 - \left( H_{r(i,j,k)}^{n-\frac{1}{2}} \right)^2 \right\} - \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^n \right)_{(i,j,k)} \]  

(A3.7b)

Finally substituting (A3.7a), (A3.7b), (A3.6a) and (A3.6b) into (A3.5), we obtain the desired expression for numerical power dissipation density at \( \text{Cube}(i,j,k) \):

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\[
\frac{1}{\Delta t} \left[ \sum_{r=x,y,z} \left( \epsilon_r(i,j,k) (E_{r(i,j,k)}^{n+1})^2 + \mu (H_{r(i,j,k)}^{n+\frac{1}{2}})^2 \right) - \Delta \left( H_{r(i,j,k)}^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right) \right] \\
- \frac{1}{\Delta t} \left[ \sum_{r=x,y,z} \left( \epsilon_r(i,j,k) (E_{r(i,j,k)}^n)^2 + \mu (H_{r(i,j,k)}^{n-\frac{1}{2}})^2 \right) - \Delta \left( H_{r(i,j,k)}^{n-\frac{1}{2}} \cdot \nabla \times E^n \right) \right] \\
+ \frac{1}{2} \left\{ \nabla \cdot \left( E^{n+1} \times H^{n+\frac{1}{2}} \right)(i,j,k) + \nabla \cdot \left( E^n \times H^{n+\frac{1}{2}} \right)(i,j,k) \right\} \\
- \frac{n^{n+\frac{1}{2}}}{P(i,j,k)} = \frac{1}{2} \left\{ \sum_{r=x,y,z} \left( E_{r(i,j,k)}^{n+1} + E_{r(i,j,k)}^n \right) H_{r(i,j,k)}^{n+\frac{1}{2}} \right\} \\
\text{(A3.8)}
\]

Equation (A3.8) only applies to a single Yee’s cell at index \((i,j,k)\). Now we determine the form for (A3.8) when sum up over all the cells. We could expand the expression in the third braces on the left-hand side of (A3.8) using (A3.2)-(A3.4). For \(E\) and \(H\) field components at \(n\) and \(n + \frac{1}{2}\) time steps:

\[
\nabla \cdot \left( E^n \times H^{n+\frac{1}{2}} \right)(i,j,k) = \nabla \cdot \left( E^n \times H^{n+\frac{1}{2}} \right)(i,j,k)_x + \nabla \cdot \left( E^n \times H^{n+\frac{1}{2}} \right)(i,j,k)_y \\
+ \nabla \cdot \left( E^n \times H^{n+\frac{1}{2}} \right)(i,j,k)_z \\
= \frac{1}{\Delta y} \left[ E^n_{x(i,j,k)} H^{n+\frac{1}{2}}_{z(i,j-1,k)} + \frac{1}{\Delta z} \right] \\
- E^n_{x(i,j,k+1)} H^{n+\frac{1}{2}}_{z(i,j,k)} \\
+ \frac{1}{\Delta x} \left[ E^n_{y(i,j,k)} H^{n+\frac{1}{2}}_{x(i,j,k-1)} + \frac{1}{\Delta z} \right] \\
- E^n_{y(i,j,k+1)} H^{n+\frac{1}{2}}_{x(i,j,k)} \\
+ \frac{1}{\Delta x} \left[ E^n_{z(i,j,k)} H^{n+\frac{1}{2}}_{y(i-1,j,k)} + \frac{1}{\Delta y} \right] \\
- E^n_{z(i,j,k+1)} H^{n+\frac{1}{2}}_{y(i,j,k)} \text{ (A3.9)}
\]

The total sum of \(\sum_{k=1}^{n_z} \sum_{j=1}^{n_y} \sum_{i=1}^{n_x} \nabla \cdot (E^n \times H^{n+\frac{1}{2}})(i,j,k)\) can be obtained by considering the sum of each component. The details are not difficult but very tedious; it will not be shown
due to lack of space. For a three-dimensional model consisting of \((n_x,n_y,n_z)\) cubes (see Figure 3.1), it can be shown that:

\[
\sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \nabla \cdot (E^n \times H^{n+1/2})_{(i,j,k)} =
\]

\[
\frac{1}{\Delta x} \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left\{ E^n_{y(n_x+1,j,k)} H^{n+1/2}_{z(n_y,j,k)} - E^n_{y(1,j,k)} H^{n+1/2}_{z(0,j,k)} \right\} +
\frac{1}{\Delta y} \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left\{ E^n_{z(i,n_y+1,k)} H^{n+1/2}_{x(i,j,k)} - E^n_{z(i,1,k)} H^{n+1/2}_{x(i,0,k)} \right\} +
\frac{1}{\Delta z} \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left\{ E^n_{x(i,j,n_z+1)} H^{n+1/2}_{y(i,j,k)} - E^n_{x(i,j,1)} H^{n+1/2}_{y(i,j,0)} \right\}
\]

Equation (A3.10) is also valid when \(E^n\) is replaced by \(E^{n+1}\). Finally by summing equation (A3.8) for all the cubes in a 3D model, we obtain the total numerical power relation:

\[
\frac{1}{2} \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left[ \sum_{r=x,y,z} \left( E^r(i,j,k) (E^{n+1}_r(i,j,k))^2 + \mu (H^{n+1}_r(i,j,k))^2 \right) - \Delta t \left( H^{n+1/2}_r \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} \right] -
\frac{1}{2} \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left[ \sum_{r=x,y,z} \left( E^r(i,j,k) (E^{n}_r(i,j,k))^2 + \mu (H^{n-1/2}_r(i,j,k))^2 \right) - \Delta t \left( H^{n-1/2}_r \cdot \nabla \times E^{n} \right)_{(i,j,k)} \right] +
\frac{\Delta t}{2} \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left[ \nabla \cdot \left( E^{n+1} \times H^{n+1/2} \right)_{(i,j,k)} + \nabla \cdot \left( E^{n} \times H^{n+1/2} \right)_{(i,j,k)} \right] =
-\Delta t \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left[ \sum_{r=x,y,z} \frac{1}{2} \left( E^{n+1}_r(i,j,k) + E^n_r(i,j,k) \right) H^{n+1/2}_r(i,j,k) \right]
\]

It is understood that (A3.10) will be used to expand the third term on the left-hand side of (A3.11). Equation (A3.11) is the finite-difference Poynting power relation for a three-dimensional FDTD model with the update equations for \(E\) and \(H\) fields.
fulfilling the canonical form of (6.2.1a)-(6.2.1f). Both (A3.10) and (A3.11) are still formidable to apply. It will be applied to a model with PEC boundary surfaces as shown in Figure 6.1. All the following E field components on the boundaries will be zero regardless of time-step n:

\[ E^n_{x(i,1,k)}, E^n_{x(i,n_x+1,k)}, E^n_{x(i,j,l)}, E^n_{x(i,j,n_z+1)} = 0 \]

\[ E^n_{y(1,j,k)}, E^n_{y(n_y+1,j,k)}, E^n_{y(i,j,l)}, E^n_{y(i,j,n_z+1)} = 0 \]

\[ E^n_{z(1,j,k)}, E^n_{z(n_z+1,j,k)}, E^n_{z(i,1,k)}, E^n_{z(i,n_y+1,k)} = 0 \]

Substituting these components into (A3.10), we observe that:

\[
\sum_{k=1}^{n_k} \sum_{j=1}^{n_j} \sum_{i=1}^{n_i} \left( \nabla \cdot \left( E^{n+1} \times H^{n+\frac{1}{2}} \right) \right)_{(i,j,k)} + \nabla \cdot \left( E^n \times H^{n+\frac{1}{2}} \right)_{(i,j,k)} = 0 \]  

(A3.12)

Thus putting (A3.12) into the numerical power relation (A3.11) yields:

\[
\frac{1}{2} \sum_{k=1}^{n_k} \sum_{j=1}^{n_j} \sum_{i=1}^{n_i} \left[ \sum_{r=x,y,z} \left( E_{r(i,j,k)} \left( E^{n+1}_{r(i,j,k)} \right)^2 + \mu \left( H^{n+\frac{1}{2}}_{r(i,j,k)} \right)^2 \right) \Delta \left( H^{n+\frac{1}{2}} \cdot \nabla \times E^{n+1} \right)_{(i,j,k)} \right] \\
- \frac{1}{2} \sum_{k=1}^{n_k} \sum_{j=1}^{n_j} \sum_{i=1}^{n_i} \left[ \sum_{r=x,y,z} \left( E_{r(i,j,k)} \left( E^n_{r(i,j,k)} \right)^2 + \mu \left( H^{n-\frac{1}{2}}_{r(i,j,k)} \right)^2 \right) \Delta \left( H^{n-\frac{1}{2}} \cdot \nabla \times E^n \right)_{(i,j,k)} \right] \\
= -\Delta t \sum_{k=1}^{n_k} \sum_{j=1}^{n_j} \sum_{i=1}^{n_i} \left[ \sum_{r=x,y,z} \frac{1}{2} \left( E^{n+1}_{r(i,j,k)} + E^n_{r(i,j,k)} \right) \right]^{n+\frac{1}{2}}_{r(i,j,k)} \\
\geq 0 \]  

(A3.13)

We observe that the left-hand side of (A3.13) consists of two expressions in similar form. The former expression contains E and H field components at time-step n + 1 and n + \(\frac{1}{2}\). The latter expression contains E and H field components at time-step n and n - \(\frac{1}{2}\). Multiplying left and right-hand side with \(\Delta V\) and calling the first expression on the left \(V^{n+1}\) and the second expression \(V^n\), (A3.13) can then be written in a compact form:

\[ V^{n+1} - V^n = \Delta t \cdot P_d \]  

(A1.14)
By expanding $V^n$ using the definitions of (A3.3) and (6.2.1g), we see that $V^n$ is similar to the definition in (6.2.2a) and $P_d$ is as given in (6.2.2b). This proves Lemma 6.1.

The following steps will derive the positive definite criteria for $V^n$. Consider the expanded expression for $V^n$:

$$V^n = \frac{dV}{2} \sum_{k=1}^{n_x} \sum_{j=1}^{n_y} \sum_{i=1}^{n_z} \left[ \sum_{r=x,y,z} \left( E_r(i,j,k)(E^n_r(i,j,k))^2 + \mu(H^n_r(i,j,k))^2 \right) \right] - H^{n-\frac{1}{2}} x(i,j,k) \left[ b_y(E^n_x(i,j,k) - E^n_y(i,j,k)) \right] - H^{n-\frac{1}{2}} y(i,j,k) \left[ b_z(E^n_x(i,j,k) - E^n_y(i,j,k)) \right] - H^{n-\frac{1}{2}} z(i,j,k) \left[ b_x(E^n_x(i,j,k) - E^n_y(i,j,k)) \right]$$  \hspace{1cm} (A3.15)

Where $b_x = \frac{\partial}{\partial x}$, $b_y = \frac{\partial}{\partial y}$ and $b_z = \frac{\partial}{\partial z}$. We could see that (A3.15) is a quadratic form, with the E and H field components constituting the variables. A quadratic expression can be written in matrix form (James 1993, Ortega 1987), for example:

$$f(x_1, x_2, x_3) = 2x_1^2 + x_2^2 + 3x_3^2 + 4x_1x_2 - 6x_1x_3 + 11x_2x_3 = [x_1 \ x_2 \ x_3]^T \begin{bmatrix} 2 & 2 & -3 \\ 2 & 1 & 11/2 \\ -3 & 11/2 & 3 \end{bmatrix} [x_1 \ x_2 \ x_3]$$

The square matrix is symmetry. When $f(x_1, x_2, x_3)$ is positive definite, $f > 0$ when $x_1$, $x_2$, $x_3 \neq 0$ and $f(0,0,0) = 0$. To show that $f(x_1, x_2, x_3)$ is positive definite, one can analyze the eigenvalues of the square matrix. Only when all the eigenvalues are greater than 0 is $f(x_1, x_2, x_3)$ positive definite (James 1994). Another approach is to apply the Sylvester’s Criteria (James 1994). Sylvester’s Criteria states that all the principal minors of the square matrix must be larger than 0 for $f(x_1, x_2, x_3)$ to be positive definite. By examining the principal minors of the matrix:
\[ P_1 = \begin{vmatrix} 2 \end{vmatrix} = 2, \quad P_2 = \begin{vmatrix} 2 & 2 \\ 2 & 1 \end{vmatrix} = -2, \quad P_3 = \begin{vmatrix} 2 & 2 & -3 \\ 2 & 1 & \frac{11}{2} \\ -3 & \frac{11}{2} & 3 \end{vmatrix} = -141.5 \]

Not all principal minors are positive, so this quadratic form is not positive definite. Both approaches are extremely difficult to apply directly to equation (A3.15) due to the large number of variables. The square matrix will be extremely large and computing its eigenvalues or principal minors will require huge computing effort. Furthermore this brute force approach is not practical, as we have to recompute the eigenvalues or principal minors every time we change the configuration of the model.

Therefore we seek an alternative method. We consider breaking the right-hand side of (A3.15) into smaller groups consisting of a few variables, with each group ideally also of quadratic form. Using Sylvester’s Criteria, conditions for each group to be positive definite are derived and by combining the conditions from all group, a general criterion can be obtained. This criterion is general in that if \( \Delta x, \Delta y, \Delta z, \Delta t, \epsilon \) and \( \mu \) of each cube fulfill the general criteria, the function \( V^n \) on the whole will be positive definite. The basis of choosing the group is that we would like the positive definite criteria to hold when there is variation of permittivity (or effective permittivity) \( \epsilon_{(i,j,k)} \) across the model. Suppose we just pay particular attention to four cubes, which are adjacent to each other, as shown in Figure A3.2.
Figure A3.2 – Four adjacent cubes.
For simplicity we assume the model to be non-magnetic $\mu_{(i,j,k)} = \mu = \mu_o$ and all cells to be similar in size. Expanding (A3.15) and just concentrating on the stored energy in the four cubes of Figure A3.2:

$$V^n = \frac{\Delta V}{2} \left\{ \sum_{r=x,y,z} \left( E_{r(i,j,k)} (E^n_{r(i,j,k)})^2 + 4 \cdot \frac{1}{4} \mu (H^{n-\frac{1}{2}}_{r(i,j,k)})^2 \right) \right\}$$

$$- H^\frac{n-1}{2}_{x(i,j,k)} \left[ b_y (E^n_{z(i,j+1,k)} - E^n_{z(i,j,k)}) - b_z (E^n_{y(i,j+1,k)} - E^n_{y(i,j,k)}) \right]$$

$$- H^\frac{n-1}{2}_{y(i,j,k)} \left[ b_z (E^n_{x(i,j+1,k)} - E^n_{x(i,j,k)}) - b_x (E^n_{z(i+1,j,k)} - E^n_{z(i,j,k)}) \right]$$

$$- H^\frac{n-1}{2}_{z(i,j,k)} \left[ b_x (E^n_{y(i,j+1,k)} - E^n_{y(i,j,k)}) - b_y (E^n_{x(i+1,j,k)} - E^n_{x(i,j,k)}) \right]$$

$$+ \sum_{r=x,y,z} \left( E_{r(i-1,j,k)} (E^n_{r(i-1,j,k)})^2 + 4 \cdot \frac{1}{4} \mu (H^{n-\frac{1}{2}}_{r(i-1,j,k)})^2 \right) \right\}$$

(A3.16)
In (A3.16), the justification for writing the H components as \(4 \cdot \frac{1}{4} \mu (H_{r(i,j,k)}^{n-\frac{1}{2}})^2\), \((r = x, y, z)\) is because each H component is surrounded or ‘shared’ by four other E field components, as seen in Figure A3.2. Also we want each group to center around an E field component. So the H field component has to be divided into four parts, each part is associated with an adjacent E field. Collecting and regrouping the terms in (A3.16) around \(E_{x(i,j,k)}^n\), \(E_{y(i,j,k)}^n\), \(E_{z(i,j,k)}^n\):

\[
V^n = \Delta V \left\{ \begin{array}{l}
\varepsilon_{x(i,j,k)} (E_{x(i,j,k)}^n)^2 + \frac{1}{4} \mu (H_{y(i,j,k)}^{n-\frac{1}{2}})^2 + \frac{1}{4} \mu (H_{y(i,j,k-l)}^{n-\frac{1}{2}})^2 \\
+ \frac{1}{4} \mu (H_{x(i,j,k)}^{n-\frac{1}{2}})^2 \\
+ \frac{1}{4} \mu (H_{x(i,j,k-l)}^{n-\frac{1}{2}})^2 \\
+ \frac{1}{4} \mu (H_{x(i,j,k-l)}^{n-\frac{1}{2}})^2 \\
& \vdots \\
\end{array} \right. 
\]

(A3.17)

In writing (A3.17) some irrelevant terms from (A3.16) have been excluded. Each expression in the braces is a group. Call the first group \(V^n_{xs}\) since its associated E field is along x-axis, \(s\) is an integer enumerating the E field index \((i,j,k)\). Proceeding to group according to all E fields in the model, (A3.17) can be written as:

\[
V^n = \Delta V \left( \sum_s V^n_{xs} + \sum_s V^n_{ys} + \sum_s V^n_{zs} \right), s = 1,2,3, \ldots 
\]

(A3.18)
By showing that each \( V^n_{xs}, V^n_{ys}, V^n_{zs} \) is positive definite, then \( V^n \) is also positive definite. Suppose we consider one of the groups centering on \( E_z \) component. Writing this as:

\[
V_z = \varepsilon E_1^2 + \frac{1}{4} \mu H_3^2 + \frac{1}{4} \mu H_1^2 + \frac{1}{4} \mu H_2^2 + \frac{1}{4} \mu H_4^2 \\
+ E_1 \left[ b_y (H_3 - H_1) - b_x (H_2 - H_4) \right]
\]

Equation (A3.19) is only applicable for interior cells, i.e. when the cell is not a boundary cell. In general to include boundary cells, the matrix \( \overline{A} \) should be generalized as:

\[
\overline{A} = \overline{A}_1 \begin{bmatrix}
\varepsilon & -\frac{1}{2} b_y & -\frac{1}{2} b_x & \frac{1}{2} b_y & \frac{1}{2} b_x \\
-\frac{1}{2} b_y & \frac{1}{4} \mu & 0 & 0 & 0 \\
-\frac{1}{2} b_x & 0 & \frac{1}{4} \mu & 0 & 0 \\
\frac{1}{2} b_y & 0 & 0 & \frac{1}{4} \mu & 0 \\
\frac{1}{2} b_x & 0 & 0 & 0 & \frac{1}{4} \mu
\end{bmatrix}
\]

\[
= \overline{x}^T \overline{A} \overline{x}
\]

Where \( a_i \in \left\{ \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{4}} \right\} \), \( i = 1,2,3,4 \). The coefficient \( a_i \) assumes these values because at the boundary cell a H field component is surrounded by two to three E field components only. This condition is illustrated in Figure A3.3.
For $V_z$ to be positive definite, the matrix $\bar{A}$ of (A3.20) must fulfills the Sylvester’s Criterion for positive definiteness. There are five principal minors $P_1, P_2, \ldots, P_5$. We begin by computing the principal minors $P_1$ and insisting that it is greater than zero, then repeating this for the other principal minors. It is implicitly assumed that $\mu > 0$.

\[ P_1 = \varepsilon > 0 \implies \varepsilon > 0 \quad (A3.21a) \]

\[ P_2 = \begin{vmatrix} \varepsilon & -\frac{1}{2}b_y & -\frac{1}{2}b_x \\ -\frac{1}{2}b_y & a_1^2\mu & -\frac{1}{4}b_y^2 \\ -\frac{1}{2}b_x & -\frac{1}{4}b_y^2 & a_1^2\mu \end{vmatrix} = a_1^2\mu\varepsilon - \frac{1}{4}b_y^2 > 0 \implies \mu \varepsilon > \frac{1}{(2a_1)^2}b_y^2 \]

Using $b_y = \frac{\Delta t}{\Delta y}$ and $c = \frac{1}{\sqrt{\mu \varepsilon}} \implies \Delta t < \frac{1}{c\frac{1}{(2a_1\Delta y)^2}}$ \quad (A3.21b)

\[ P_3 = \begin{vmatrix} \varepsilon & -\frac{1}{2}b_y & -\frac{1}{2}b_x \\ -\frac{1}{2}b_y & a_1^2\mu & 0 \\ -\frac{1}{2}b_x & 0 & a_2^2\mu \end{vmatrix} = (a_1a_2\mu)^2\varepsilon - \mu\left(a_1b_x\right)^2 - \frac{\mu}{4}\left(a_2b_y\right)^2 > 0 \]

\[ \implies \mu \varepsilon > \left(\frac{b_x}{2a_2}\right)^2 + \left(\frac{b_y}{2a_1}\right)^2 \implies \Delta t < \frac{1}{c\sqrt{\frac{1}{(2a_2\Delta x)^2} + \frac{1}{(2a_1\Delta y)^2}}} \quad (A3.21c) \]
\[
P_4 = \begin{bmatrix}
\varepsilon & -\frac{1}{2} b_y & -\frac{1}{2} b_x & -\frac{1}{2} b_y \\
-\frac{1}{2} b_y & a_1^2 \mu & 0 & 0 \\
-\frac{1}{2} b_x & 0 & a_2^2 \mu & 0 \\
\frac{1}{2} b_y & 0 & 0 & a_3^2 \mu
\end{bmatrix} = (-1)^{1+4} \begin{bmatrix}
-\frac{1}{2} b_y & a_1^2 \mu & 0 \\
-\frac{1}{2} b_x & 0 & a_2^2 \mu \\
\frac{1}{2} b_y & 0 & 0
\end{bmatrix} + (-1)^{4+4} a_3^2 \mu P_3 > 0
\]

\[
\Rightarrow \left( \frac{a_1 a_2}{2} \mu b_y \right)^2 + \left( a_3^2 \mu \right) P_3 > 0 \Rightarrow \mu \epsilon > \left( \frac{b_x}{2a_2} \right)^2 + \left( \frac{b_y}{2a_4} \right)^2 + \left( \frac{b_y}{2a_3} \right)^2
\]

\[
\Rightarrow \Delta t < \frac{1}{c} \sqrt{\frac{1}{(2a_2 \Delta x)^2} + \frac{1}{\left( a_1 a_3 \right)^2 a_y^2}}
\]

\[
P_5 = \begin{bmatrix}
\varepsilon & -\frac{1}{2} b_y & -\frac{1}{2} b_x & -\frac{1}{2} b_y \\
-\frac{1}{2} b_y & a_1^2 \mu & 0 & 0 \\
-\frac{1}{2} b_x & 0 & a_2^2 \mu & 0 \\
\frac{1}{2} b_y & 0 & 0 & a_3^2 \mu \\
\frac{1}{2} b_x & 0 & 0 & a_4^2 \mu
\end{bmatrix} = (-1)^{1+5} \begin{bmatrix}
-\frac{1}{2} b_y & a_1^2 \mu & 0 & 0 \\
-\frac{1}{2} b_x & 0 & a_2^2 \mu & 0 \\
\frac{1}{2} b_y & 0 & 0 & a_3^2 \mu \\
\frac{1}{2} b_x & 0 & 0 & a_4^2 \mu
\end{bmatrix} + (-1)^{5+5} a_4^2 \mu P_4 > 0
\]

\[
\Rightarrow \mu \epsilon > \left( \frac{b_x}{2a_2} \right)^2 + \left( \frac{b_x}{2a_4} \right)^2 + \left( \frac{b_y}{2a_3} \right)^2 + \left( \frac{b_y}{2a_3} \right)^2
\]

\[
\Rightarrow \Delta t < \frac{1}{c} \sqrt{\frac{1}{\left( \frac{2a_3 a_4}{a_2^2 + a_4^2} \right)^2 \Delta x^2} + \frac{1}{\left( \frac{2a_1 a_3}{\sqrt{a_1^2 + a_3^2}} \right)^2 \Delta y^2}}
\]

From (A3.21a) to (A3.21e), we see that \( \mu > 0, \epsilon > 0 \) and \( \Delta t \) needs to be smaller than a certain limit. The smallest limit from (A3.21b) to (A3.21e) for all combination of \( a_1, a_2, a_3 \) and \( a_4 \) will be taken as the constraint for \( \Delta t \). Table A3.1 shows the values for the coefficient of \( \Delta x \) and \( \Delta y \) for different combinations of \( a_1, a_2, a_3 \) and \( a_4 \).
Consider the expression:

\[
\frac{1}{\sqrt{(c_1\Delta x)^2 + (c_2\Delta y)^2}} = \frac{1}{\sqrt{\frac{1}{c_1^2} \left(\frac{1}{\Delta x^2}\right) + \frac{1}{c_2^2} \left(\frac{1}{\Delta y^2}\right)}}
\]

The smallest value is obtained when the denominator is maximum. If \(\Delta x\) and \(\Delta y\) are fixed, then \(c_1\) and \(c_2\) must be as small as possible. Using Table A3.1, we observe that:

\[
\frac{1}{\sqrt{(2a_1\Delta y)^2}} > \frac{1}{\sqrt{(2a_2\Delta x)^2}} \quad \frac{1}{\sqrt{(2a_2\Delta x)^2}} > \frac{1}{\sqrt{(2a_2\Delta y)^2}}
\]

Also from Table A3.1, we observe that \(\frac{2a_1a_3}{\sqrt{a_1^2 + a_3^2}}\) and \(\frac{2a_2a_4}{\sqrt{a_2^2 + a_4^2}}\) are smallest when \(a_1 = a_3 = a_2 = a_4 = \frac{1}{\sqrt{4}}\). The corresponding coefficients for \(\Delta x\) and \(\Delta y\) are \(\frac{1}{\sqrt{2}}\). We conclude that if \(\Delta t\) satisfies:
\begin{align*}
\Delta t < \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}} = \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}}, \quad c = \frac{1}{\sqrt{\mu \varepsilon}} \quad (A3.23a)
\end{align*}

Then all conditions of (A3.21b) to (A3.21e) will be fulfilled and \( V_z \) will be positive definite. This procedure can also be applied to \( V_x \) and \( V_y \), whose details would not be provided:

For \( V_x \): \( \Delta t < \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}} \)  
For \( V_y \): \( \Delta t < \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}} \) \quad (A3.23b)

Equations (A3.23a) and (A3.23b) apply to a single cell. To ensure that all groups \( V^n_{xs} \), \( V^n_{ys} \) and \( V^n_{zs} \), \( s \in \{1,2,3\cdots\} \) in the 3D model are positive definite, these need to be enforced for every cell. This requirement can be summarized as follows:

For a 3D FDTD model according to Yee’s formulation, suppose the followings apply:

1. Update equations for E and H field components are given by the Canonical FDTD Form (6.2.1a) to (6.2.1f).
2. Boundaries of the model are perfect electric conductor (PEC).
3. All cubes are similar in size with edges \( \Delta x, \Delta y \) and \( \Delta z \).

Then for all \( i \in \{1,2,\cdots,n_x\}, j \in \{1,2,\cdots,n_y\}, k \in \{1,2,\cdots,n_z\} \), \( \Delta V = \Delta x\Delta y\Delta z \), the function:

\[
V^n = \frac{\Delta V}{2} \sum_{k=1}^{n_z} \sum_{j=1}^{n_y} \sum_{i=1}^{n_x} \left[ \sum_{r=x,y,z} \left( \varepsilon_r(i,j,k)(E^n_r(i,j,k))^2 + \mu(H^{n-\frac{1}{2}}_r(i,j,k))^2 \right) - \Delta t \left( H^{n-\frac{1}{2}}_r \cdot \nabla \times E^n \right)_{(i,j,k)} \right]
\]

is positive definite if and only if:

- \( \varepsilon_x(i,j,k) > 0, \varepsilon_y(i,j,k) > 0, \varepsilon_z(i,j,k) > 0 \) and \( \mu > 0 \).

- For \( \varepsilon = \min\{\varepsilon_x(i,j,k), \varepsilon_y(i,j,k), \varepsilon_z(i,j,k)\} \) and \( c_m = \frac{1}{\sqrt{\mu \varepsilon}} \), let:

\[
\Delta t < \min \left\{ \frac{1}{c_m \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}}, \frac{1}{c_m \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta z^2}}}, \frac{1}{c_m \sqrt{\frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}} \right\}
\]

This proves Lemma 6.2.
Appendix 4 - Stability for Three-Dimensional FDTD Model

We now prove Theorem 6.3. Suppose a FDTD framework satisfies all the conditions of Lemma 6.1 and 6.2. Since $V^n$ is positive definite, it can be written in the form:

$$V^n = \overline{X}^T \overline{P} \overline{X} , \quad \overline{X} \in \mathbb{R}^M$$  \hspace{1cm} (A4.1)

where $\overline{X}$ is given by (6.2.5a) and $M$ is as given by (6.2.5b) and $\overline{P}$ is a square symmetric matrix of order $M$. Superscript $T$ represents matrix transposition.

Introducing the linear transformation $\overline{X} = \overline{Q} \overline{Y}$:

$$V^n = \overline{Y}^T \left( \overline{Q} \overline{P} \overline{Q} \right) \overline{Y}$$  \hspace{1cm} (A4.2)

The matrix transformation $\overline{Q} \overline{P} \overline{Q}$ of (A4.2) is a special form of Similarity Transformation known as Congruence Transformation (Ortega 1987). Since matrix $\overline{P}$ is positive definite, from linear algebra we know that a nonsingular matrix $\overline{Q}$ exists such that (Ortega 1987, chapter 3):

$$\overline{P} = \text{diag}(1,1,\ldots,1)$$

Thus

$$V^n = \overline{Y}^T \left( \overline{Q} \overline{P} \overline{Q} \right) \overline{Y} = \overline{Y}^T \overline{P} \overline{Y} = y_1^2 + y_2^2 + y_3^2 + \cdots + y_M^2$$  \hspace{1cm} (A4.3)

Taking an arbitrary norm for $\overline{Y} = \overline{Q}^{-1} \overline{X}$:

$$\|\overline{Y}\| = \left\| \overline{Q}^{-1} \overline{X} \right\| \leq \left\| \overline{Q}^{-1} \right\| \|\overline{X}\|$$  \hspace{1cm} (A4.4)

Where $\left\| \overline{Q}^{-1} \right\|$ is a finite positive value called the matrix or operator norm as defined in (Ortega 1987, chapter 2). We thus have the following implication from (A4.4):

$$\|\overline{Y}\| \to \infty \Rightarrow \|\overline{X}\| \to \infty$$  \hspace{1cm} (A4.5)

Observe that from (A4.3), $V^n = \overline{X}^T \overline{P} \overline{X} = \overline{Y}^T \overline{Y}$ is radially unbounded (Khalil 1996, chapter 3) in relation to elements of $\overline{Y}$. This means that if $V^n$ approaches infinity, at
least one of the elements of \( \bar{Y} \) must also approaches infinity. Suppose we use the \( L_2 \) vector norm:

\[
\|\bar{X}\| = \left( x_1^2 + x_2^2 + \cdots + x_M^2 \right)^{\frac{1}{2}} \quad \text{and} \quad \|\bar{Y}\| = \left( y_1^2 + y_2^2 + \cdots + y_M^2 \right)^{\frac{1}{2}}
\]

(A4.6)

Using (A4.5) we note that \( V^n \) is also radially unbounded in relation to elements of \( \bar{X} \). This implies that if \( V^n \) is bounded, all the elements in \( \bar{X} \) must also be finite, i.e. all the \( E \) and \( H \) field components are finite. For \( V^n \) to be bounded for \( n = 1, 2, 3, \ldots \), a sufficient condition is \( P_d \) be negative or zero. This completes the proof.
Appendix 5 – Negative Region For Resistive Voltage Source

We first note from Piket-May 1994 that to derive equation (6.4.1) the current of a resistive voltage source is:

\[
I_s^{n+\frac{1}{2}} = \frac{\Delta t}{2R_s} (E_z^n + E_z^{n+1}) + \frac{V_i^{n+\frac{1}{2}}}{R_s} \tag{A5.1}
\]

From \( \nabla \times \vec{H} = \vec{J} + e \frac{\partial \vec{E}}{\partial t} \) and using center difference scheme according to Yee’s formulation, concentrating on z component of E field at \((i,j,k)\) (assuming the source to coincide with \(E_z(i,j,k)\)):

\[
\nabla \times H_z^{n+\frac{1}{2}}(i,j,k) = \frac{I_s^{n+\frac{1}{2}}}{\Delta x \Delta y} + \frac{\varepsilon}{\Delta t} \left( E_z^{n+1}(i,j,k) + E_z^n(i,j,k) \right) \tag{A5.2}
\]

Let \( V_s^{n+\frac{1}{2}} \) be a constant, called it \( V_{so} \) and limiting the maximum source current to \( I_s^{(max)} = \frac{V_{so}}{R_s} \). Let us also introduce the notations \( x = E_z^n(i,j,k), \ x^{n+1} = E_z^{n+1}(i,j,k), \)

\( y = \nabla \times H_z^{n+\frac{1}{2}}(i,j,k), \ v = \frac{V_{so}}{\Delta z} \). Then from (A5.2):

\[
\frac{\Delta t}{\varepsilon} \nabla \times H_z^{n+\frac{1}{2}}(i,j,k) - (E_z^{n+1}(i,j,k) + E_z^n(i,j,k)) = \frac{\Delta t I_s^{n+\frac{1}{2}}}{\varepsilon \Delta x \Delta y} < 2 \frac{\Delta t \Delta z}{2\varepsilon \Delta x \Delta y \Delta z} \frac{V_{so}}{\Delta z} = 2D_z v
\]

\[\Rightarrow \ y < \frac{2\varepsilon}{\Delta t} D_z v + \frac{\varepsilon}{\Delta t} \left( x^{n+1} - x \right) \tag{A5.3} \]

where \( D_z = \frac{\Delta t \Delta z}{2\varepsilon \Delta x \Delta y} \). Substituting (6.4.1) for \( x^{n+1} = E_z^{n+1}(i,j,k) \) into inequality (A5.3), and performing some algebra:

\[ y < \frac{2\varepsilon}{\Delta t} D_z v + \frac{\varepsilon}{\Delta t} + \frac{1}{2} D_z \left( \frac{\Delta t}{\varepsilon} y - 2D_z (x + v) \right) \]

\[ \Rightarrow \ y < \frac{2\varepsilon}{\Delta t} (D_z v - x) \tag{A5.4} \]

The intersection of region described by (A5.4) and region A of Figure 6.7 is shown in Figure A5.1. We call this region C. From Figure A5.1, we notice that in order for the resistive voltage source to be continuously supplying energy to the model, the new value for \( x^{n+1} = E_z^{n+1}(i,j,k) \) must be greater than \(-v\). Otherwise there is no chance the elemental dissipation can be negative. Thus enforcing this requirement from (6.4.1):
\[ x^{n+1} = \frac{1-D_z}{1+D_z} x + \frac{\Delta_t}{\varepsilon(1+D_z)} y - \frac{2D_z}{1+D_z} v > -v \]

\[ \Rightarrow y > -\frac{\varepsilon}{\Delta_t} (1-D_z)(x+v) \]  

\[ (A5.5) \]

(A5.4), (A5.5) and \( D^{n+\frac{1}{2}}(x,y,v) \leq 0 \) corresponds to the (6.4.4a)-(6.4.4c). Using these inequalities, the region of Figure 6.8A can be generated for \( D_z < 1 \). Inequality (A5.5) will degenerate to \( y = 0 \) when \( D_z > 1 \), allowing us to generate Figure 6.8B.

![Figure A5.1](image)

**Figure A5.1** – Intersection of \( D^{n+\frac{1}{2}}(x,y,v) \leq 0 \) and \( y < \frac{2\varepsilon}{\Delta_t} (D_zv - x) \)