The purpose of boundary conditions in FDTD is to prevent the reflection at the boundary (end of the model). For our 1D case, this will be the left and right sides.

Need more complete reference material for these notes? See the Taflove paper linked to the website.

Start with the Wave Equation. This assumes the waves hitting the boundary are outgoing spherical waves. This is a good approximation “far” from an object. U is any field (E or H). For the 1D TE-to-z case, this will be Ey.

\[
\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\right)U = 0
\]

This can be written in 2D

\[
U_{xx} + U_{yy} - \frac{U_{tt}}{c^2} = 0
\]

where

\[
U_{xx} = \frac{\partial^2 E}{\partial x^2}, \text{etc.}
\]

\(U\) sin g operator notation :

\(LU = 0\)

where

\(L = D_x^2 + D_y^2 - D_t^2\)

and

\(D_x^2 = \frac{\partial^2}{\partial x^2}, D_y^2 = \frac{\partial^2}{\partial y^2}, D_t^2 = \frac{1}{c^2} \frac{\partial^2}{\partial t^2}\)

This can be factored into + and - traveling waves:
\[ LU = L^+ L^- U = 0 \]

where

\[ L^- = D_x - D_t \sqrt{1 - S^2} \]
\[ L^+ = D_x + D_t \sqrt{1 - S^2} \]
\[ S = \frac{D_y}{D_t} \]

Enquist and Majda show that a \(-x\) traveling wave will be absorbed at the left hand boundary if:

\[ L^- U = 0 \quad @ \quad x = 0 \]

This is EXACT. No approximations are made, yet. If you find \( U \) such that \( L^- U = 0 \), then the wave will be perfectly absorbed. None will reflect.

For discrete programming (such as FDTD)
APPROXIMATIONS of \( L^- \) are made:

First Order: (using Taylor Expansion)

\[ \sqrt{1 - S^2} \approx 1 \]
\[ L^- \approx \frac{\partial}{\partial x} - \frac{1}{c_o} \frac{\partial}{\partial t} \]
\[ \left( \frac{\partial}{\partial x} - \frac{1}{c_o} \frac{\partial}{\partial t} \right) U \bigg|_{x=0} = 0 \]

The amount of field that reflects at the boundary depends on the direction of propagation of the wave:
\[ \Gamma = \frac{\cos(\theta) - 1}{\cos(\theta) + 1} \]

\[ = 0\% \text{ for normal incidence (}\theta = 90^\circ\text{)} \]

\[ \approx 17\% \text{ for } 45^\circ \text{ incidence} \]

So, for our 1D case, the first order Mur boundary condition is ‘perfect.’ The only source of error is numerical roundoff.

**Second Order:**

\[ \sqrt{1 - S^2} \approx 1 - \frac{S^2}{2} \]

\[ \mathcal{L} \approx \frac{\partial}{\partial x} - \frac{1}{c_o} \frac{\partial}{\partial t} \left( 1 - \frac{1}{2} \left( \frac{\partial}{\partial y} \left( \frac{1}{c_o} \frac{\partial}{\partial t} \right) \right)^2 \right) \]

Multiply \( \mathcal{L} \) by \( \frac{1}{c_o} \frac{\partial}{\partial t} \)
$L^{-} \approx \frac{1}{c_{o}^{2}} \frac{\partial^{2}}{\partial x \partial t} - \frac{1}{c_{o}^{2}} \frac{\partial^{2}}{\partial t^{2}} + \frac{1}{2} \frac{\partial^{2}}{\partial y^{2}}$

\[
\left( \frac{1}{c_{o}^{2}} \frac{\partial^{2}}{\partial x \partial t} - \frac{1}{c_{o}^{2}} \frac{\partial^{2}}{\partial t^{2}} + \frac{1}{2} \frac{\partial^{2}}{\partial y^{2}} \right) U \bigg|_{x=0} = 0
\]

$\Gamma = \left| \frac{\cos(\theta) - 1}{\cos(\theta) + 1} \right|^{2}$

$= 0\%$ for normal incidence \\
$= 3\%$ for $\theta = 45^\circ$

Both the 1st and 2nd order “MUR” boundary conditions are approximations, and are therefore not perfect.

The amount of error depends on
- the angle of incidence (see gamma)
- the cell size and frequency (numerical error in differentiation)

How are these programmed in FDTD? 
Apply numerical differentiation to derivatives.

Spatial Derivative (d/dx): Taking the central difference will give a derivative defined at Ez(1/2)

*   *   *   \rightarrow x \\
Ez(1) Ez(1.5) Ez(2)

Time derivative (d/dt): Taking the central difference will give a derivative defined at Ez$^{n+1/2}$

*   *   *   \rightarrow t \\
Ez$^{n}$(i) Ez$^{n+1/2}$(i) Ez$^{n+1}$(i)

All parts of the equation must be defined at the same location ($x = \frac{1}{2}$) and time ($n+1/2$). This will require some averaging, just as our original FDTD code did.
Here is the \( L^+ U = 0 \) boundary condition for the LEFT boundary:

\[
\left( \frac{\partial}{\partial z} - \frac{1}{c_o} \frac{\partial}{\partial t} \right) E_y = 0
\]

Apply at \( t = n + 1/2, x = 1/2 \)

\[
\begin{bmatrix}
\frac{E_y^{n+1}(2) - E_y^{n+1}(1)}{d_z} + \frac{E_y^n(2) - E_y^n(1)}{d_z}
\end{bmatrix}
\begin{bmatrix}
\frac{1}{2} \frac{dt}{c_o}
\end{bmatrix}
- \frac{1}{c_o} \begin{bmatrix}
\frac{E_y^{n+1}(2) - E_y^n(2)}{dt} + \frac{E_y^{n+1}(1) - E_y^n(1)}{dt}
\end{bmatrix} = 0
\]

Solve for \( E_y^{n+1}(1) \)

\[
E_y^{n+1}(1) = E_y^n(2) + \frac{c_o dt - d_z}{c_o dt + d_z} \left[ E_y^{n+1}(2) - E_y^n(1) \right]
\]

Here is an example of how I programmed the FDTD Boundary conditions. Put these statements AFTER you have calculated the E fields and before you calculate H:

```plaintext
RBC_const = (vp*dt-dx)/(vp*dt+dx) % Mur 1st order
ey(1) = eyold_2 + RBC_const*(ey(2) - eyold_1)
eyold_1 = ey(1)
eyold_2 = ey(2)
```

For the RIGHT side, repeat this analysis with \( L^+ U = 0 \). You should get:

\[
E_y^{n+1}(nx) = E_y^n(nx-1) + \frac{c_o dt - d_z}{c_o dt + d_z} \left[ E_y^{n+1}(nx-1) - E_y^n(nx) \right]
\]

(where \( nx \) is the integer for the RIGHT boundary location)

Note that we only have to do the boundary condition on one of the fields (E or H) at the boundary. We have chosen E, but we could just as well have chosen H. The other field will be calculated using regular FDTD.

**PRACTICAL APPLICATION:**

Assumptions made:

- waves hitting boundary are outgoing spherical waves. (started with the wave equation)
  - Good approximation far from the object
How far is far? ½ wavelength is rule-of-thumb

Practical Application: This RBC works well to within 1/8 wavelength, except for “strong” sources/scatterers like antenna feedpoints.

Describe scattered field/total field combination simulation used by Taflove and others

• 1st or second order approximation to operator
  • Reflection coefficient depends on angle of incidence
  • CORNERS are bad. Have to be handled specially, and bulk of error comes from corners

• Numerical Differentiation
  • Reflection depends on cell size and frequency
  • 2nd order Mur is generally used in practice.

• Mur 2nd order RBC is commonly used in most applications.

• Other RBCs
  • Retarded Time. Assume a plane wave hitting the boundary (as opposed to a spherical wave). Gives simpler difference equations, and approximately the same accuracy as Mur.
  • PML. Use a series of “active materials” to absorb the wave. Since FDTD is physically modeling what the wave does, this is what would happen if you built a room out of a series of layers of absorbing material, and sent a wave into it.
  • Higher Order RBCs. Sometimes used, but PML has them “beat”
  • Adaptive RBCs. PML generally better, unless you know something (apriori) about the wave hitting the boundary, such as in waveguide analysis.