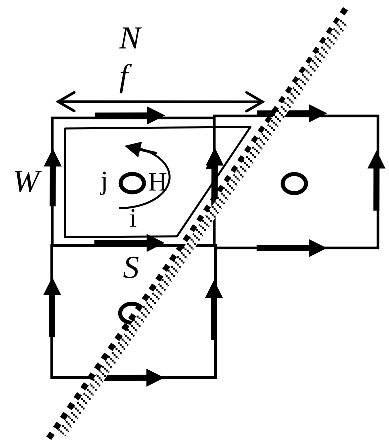
Modeling: Absorbing boundary conditions; dispersive material; fixes for staircasing
Book Ch. 5.3 pp 79- 81

1 Fixes for staircasing

The square Yee cells cannot represent curved material interfaces well – the “staircasing” or “LEGO” effect. Proper resolution of boundaries can be achieved by e.g. unstructured grids and finite elements. Usually one combines the Yee staggered grid in “free space” with finite elements near boundaries into a “hybrid” scheme. A.Bondeson (one of the authors of the book) showed how the combination can be done to make a stable method.
Here we will briefly introduce improvements in the FDTD spirit for non-grid aligned boundaries a) at PEC and b) at dielectric interfaces.

1.1 Non-aligned PEC boundaries



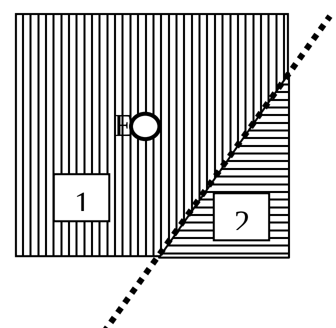
The Yee scheme can be derived from Faraday’s law by line integrals and the Stokes’ theorem. Suppose a PEC boundary cuts the cells as shown right. The line integral around the skewed quadrilateral with area *A* gets no contribution from the PEC part: the tangential component is zero there, and we obtain (TM case)

$$\mu\int_A \frac{\partial H}{\partial t}dxdy = -\oint_C \mathbf{E}\bullet d\mathbf{l}$$

$$\mu A\frac{dH}{dt} = \Delta y E_y^W + fE_x^N - g\cdot E_x^S$$

etc. where f and g are the lengths of grid-lines cut by the boundary. Note that there are several cases for how the boundary cuts the cell, and rules-of-thumb are needed to choose e.g. which cells to keep. There are also stability issues. Still such modifications do improve the accuracy.

1.2 Non-aligned Dielectric boundaries



Dey and Mittra devised a simple scheme of area (volume- in 3D) – weighting:

$$\varepsilon_{eff}\frac{d\mathbf{E}_{ij}}{dt} = (\nabla\times\mathbf{H})_{ij}, \varepsilon_{eff} = \frac{\varepsilon_1 A_1 + \varepsilon_2 A_2}{A_1 + A_2}$$

2 Dispersive material

Most real materials have properties that depend on the frequency ω of the illumination. They can often be well modeled in the frequency domain by ε(ω), etc. and in the time domain by a convolution, (the hat denotes the phasor, or Fourier coefficient)

$$D = \varepsilon_0(\varepsilon_\infty E + \int_0^t E(t-\tau)\chi(\tau)d\tau) : \hat{D}(\omega) = \varepsilon_0(\varepsilon_\infty + \hat{\chi}(\omega))\hat{E}(\omega)$$

If the transform of the impulse response function χ can be well approximated by a rational function, the convolution can be computed by an "ADE" – an augmented set of differential equations. As an example, take a "single pole Debye" material,

$$\hat{\chi}(\omega) = \frac{\Delta\varepsilon}{1 + j\omega\tau} \text{ which becomes } \chi(t) = \frac{\Delta\varepsilon}{\tau_P} e^{-t/\tau_P}$$

in the time domain. The frequency domain (E,D)-relation is

$$D(\omega) = \varepsilon_0 (\varepsilon_\infty + \frac{\Delta\varepsilon}{1 + j\omega\tau_P}) E(\omega)$$

and in time domain

$$D + \tau_P \frac{dD}{dt} = \varepsilon_0 (E + \tau_P \frac{dE}{dt} + \Delta\varepsilon E)$$

There remains to see how this plays out in the Yee-scheme for the Maxwell equations

$$\nabla \times \hat{H} = \varepsilon_0 (\varepsilon_\infty + \frac{\Delta\varepsilon}{1 + j\omega\tau_P}) \hat{E} + \sigma\hat{E} = \varepsilon_0 \varepsilon_\infty V + \sigma\hat{E} + \hat{J}, \hat{J} = \frac{\varepsilon_0 \cdot \Delta\varepsilon}{1 + j\omega\tau_P} \hat{E}$$

so the time-domain equation including the J-current is

$$\begin{cases} \nabla \times H = \varepsilon_0 \varepsilon_\infty \dfrac{\partial E}{\partial t} + \sigma E + J \\ \tau_P \dfrac{dJ}{dt} + J = \varepsilon_0 \Delta\varepsilon \dfrac{dE}{dt} \end{cases}$$

In the Yee-discretization we let J share gridpoints with E:

$$\begin{cases} \tau_P \dfrac{J^{n+1} - J^n}{\Delta t} + \dfrac{J^{n+1} + J^n}{2} - \varepsilon_0 \varepsilon_\infty \dfrac{E^{n+1} - E^n}{\Delta t} = 0 \\ \varepsilon_0 \varepsilon_\infty \dfrac{E^{n+1} - E^n}{\Delta t} + \sigma \dfrac{E^{n+1} + E^n}{2} + \dfrac{J^{n+1} + J^n}{2} = (\nabla \times H^{n+1/2}) \end{cases}$$

which is a 2x2 linear system to solve, always non-singular. *Exercise: Show!*

3 Absorbing boundary conditions: ABC

For simulations, the Yee grid must be terminated by boundary conditions. If we let E-points be the extreme gridpoints, the obvious choice is to set E to zero there: a PEC boundary. For TE waves one may choose a grid with H-points at the edges and terminate by a PMC (perfect magnetic conductor). But PEC boundaries are perfect reflectors, and their reflections will disturb the signals in the object under study. The design of efficient non-reflective conditions has proceeded along two lines: Analytic ABC, e.g. the "Mur" conditions implemented in Lab 1, were developed first, favored by numerical analysts for the intricate stability analysis required, and use the hyperbolic properties (characteristics, etc,) of the Maxwell equations. Engineers have often used instead a damping layer with lossy material next to the exterior PEC boundary to absorb the waves so that very little reaches it. The walls of anechoic chambers are covered with porous spikes to provide the damping, With the Perfectly Matched Layer invented by P.Berenger around 1990 the battle between the two types was over: PML is more robust and achieves higher damping over a larger set of incidence angles. The design of stealth aircraft was one of the drivers for better ABC. When the radar cross section is the size of a crow, spurious reflections from exterior boundaries must be annihilated lest they swamp the signals from the object.

3.1 Analytical ABC

We show the simplest case here, for the scalar wave equation $u_{tt} = c^2 u_{xx}$. Suppose we wish to let waves out to the right at $x = L$. The general solution (d’Alembert) of the wave equation is described as the sum of a right-running wave f and a left-running wave g.

$$u = f(x - ct) + g(x + ct)$$

Clearly, the *left*-running wave is also a solution of the one-way wave equation

$u_t + cu_x = 0$ (and the right-running: $u_t - cu_x = 0$)

and this can be used as a numerical absorbing condition.
For waves along the x-axis it is perfect for the continuous model. After discretization it is less perfect (dispersion, again) but simple and accurate enough for many applications.
The Mur condition is simply a discretization in the Yee spirit of the one-way equation. Two formulations are suggested in the Lab1 handout.
The lecture notes “ABCetc” go on to calculate the reflection coefficient of the one-way condition in a 2D setting, and then give a short presentation of improved versions, the Engquist-Majda family, which is much better for a larger range of incidence angles.

The Berenger PML splits the fields (every component) into normal to the absorbing wall and tangential to it, and adds damping only to the normal component. Efficient and big step forward, in theory, but painstaking coding: there are twelve Maxwell components, and different models on walls in x, y, and z, and wedges ad corners of the rectangular grid brick have to be treated specially.

3.2 UPML

The Uniaxial PML (UPML) is much easier to implement and employs no field splitting. It does, as we shall see, introduce new differential equations, but of the benign type we saw for the modeling of dispersive materials.
The initial idea is this: Look at the lossy Faraday’s law. It could be derived from a *non*-lossy material by a “stretching” of the space variables, $dx_1 = s_x\, dx$, by a *complex* scale factor s_x. This, again, is equivalent to a modification of the isotropic material into an orthotropic one, so we wind up with diagonal permittivity and permeability tensors,

$$\varepsilon\begin{pmatrix}\varepsilon_1 & 0 & 0\\ 0 & \varepsilon_2 & 0\\ 0 & 0 & \varepsilon_3\end{pmatrix}, \mu\begin{pmatrix}\mu_1 & 0 & 0\\ 0 & \mu_2 & 0\\ 0 & 0 & \mu_3\end{pmatrix}$$

We will now show that a material interface, assumed normal to the x-axis, between a homogeneous material with $\varepsilon_i = \mu_i = 1$ and the damping layer can be made *exactly* free of reflections for any incidence angles, any frequencies, etc., by proper choice of ε_i and μ_i. This is surely surprising, and also the very simple final result on *how* to choose the ε_i and μ_i.

Let the interface be $x = 0$, $x < 0$ is the non-lossy isotropic part and $x > 0$ is the anisotropic layer. We consider TM waves, so the incoming wave is $E_z = \exp(j(k_1 x + k_2 y))$ with $\mathrm{Re}k_1 < 0$ and this is the total field in $x < 0$ since there is to be *NO REFLECTED* wave. In $x > 0$, let the wave be $E_z = T\exp(j(\kappa_1 x + \kappa_2 y))$ with Re $\kappa_1 < 0$ so the wave moves away from the interface. Note that κ_i can be complex but k_i are real. The interface conditions are that the tangential components E_z and H_y be continuous.

The Maxwell equations are

$$\begin{aligned} \varepsilon\varepsilon_3 j\omega E_z &= \partial_y H_x - \partial_x H_y \\ \mu\mu_1 j\omega H_x &= \partial_y E_z \\ \mu\mu_2 j\omega H_y &= -\partial_x E_z \end{aligned} \quad \text{or for the plane wave,} \quad \begin{aligned} \varepsilon\varepsilon_3 \omega E_z &= \kappa_y H_x - \kappa_x H_y \\ \mu\mu_1 \omega H_x &= \kappa_y E_z \\ \mu\mu_2 \omega H_y &= -\kappa_x E_z \end{aligned}$$

From this follows the dispersion relation,

$$\varepsilon\mu\varepsilon_3\omega^2 = \frac{\kappa_x^2}{\mu_2} + \frac{\kappa_y^2}{\mu_1}$$

and the continuity requirements, including phase matching for every y across $x = 0$,

$$[E_z] = 0: \quad \exp(jk_y y) = T\exp(jk_y y): k_y = \kappa_y, T = 1$$

$$[H_y] = 0: \quad jk_x \exp(jk_y y)/1 = j\kappa_x T\exp(j\kappa_y y)/\mu_2 : k_x = \kappa_x/\mu_2$$

Replacing the κ in the dispersion relation by the expressions on k we obtain

$$\varepsilon\mu\varepsilon_3\omega^2 = \mu_2 k_x^2 + \frac{k_y^2}{\mu_1} \qquad (*)$$

If we choose

$$\varepsilon_3 = \mu_2 = 1/\mu_1$$

(*) is satisfied for all k with $\varepsilon\mu\omega^2 = k_x^2 + k_y^2$ which is true for all incidence angles and all frequencies ω!

In 3D the two materials are perfectly matched across the interface if

$$\varepsilon_i = \mu_i = \frac{s_1 s_2 s_3}{s_i^2}, i = 1,2,3$$

For an x-interface choose $s_2 = s_3 = 1$, y-interface: $s_1 = s_3 = 1$ and a z-interface $s_1 = s_2 = 1$

3.2.1 Choice of *s* and the 1D (transmission line) case

Now we proceed to choose s to produce damping. Look at a 1D case with resistive damping,

$$\varepsilon j\omega E_z + \sigma E_z = -\partial_x H_y : \varepsilon j\omega(1 + \frac{\sigma}{\varepsilon j\omega})E_z = -\partial_x H_y$$

so $s_1 = 1/s_3 = 1/s_2 = (1 + \dfrac{\sigma}{\varepsilon j\omega})$, and the Maxwell equations become

$$\varepsilon j\omega(1+\frac{\sigma}{\varepsilon j\omega})E_z = -\partial_x H_y : \varepsilon\partial_t E_z + \sigma E_z = -\partial_x H_y$$

$$\mu j\omega(1+\frac{\sigma}{\varepsilon j\omega})H_y = -\partial_x E_z : \mu\partial_t E_z + \sigma^* E_z = -\partial_x E_z, \sigma^* = \frac{\mu\sigma}{\varepsilon}$$

We recognize the condition as *impedance* matching: the wave impedance $Z = H/E$ satisfies

$$Z = \frac{\varepsilon j\omega + \sigma}{\mu j\omega + \sigma^*}\cdot\frac{1}{Z}; Z^2 = \frac{\varepsilon j\omega + \sigma}{\mu j\omega + \frac{\mu\sigma}{\varepsilon}} = \frac{\varepsilon}{\mu}, Z = \pm\sqrt{\frac{\varepsilon}{\mu}}$$

which is real and the same as in the non-lossy domain (+-: left- and right-running waves). The Lab 1 final exercise produces the UPML boundary condition in this way.
In 1D there is no need for a whole damping layer: A transmission line can be terminated with no reflections by an impedance matched resistor. All we need is

$$E = \pm\sqrt{\frac{\mu}{\varepsilon}}H = \pm\sqrt{\frac{\mu}{\varepsilon}}\cdot -\frac{j\varepsilon\omega}{jk}E; \; jkE = \mp\sqrt{\varepsilon\mu}\cdot j\omega E :$$

$$\partial_t E \pm c\partial_x E = 0$$

which (of course …) is the Mur or Characteristic ABC re-discovered, - for left-running waves and + for right-running. But in 2D and 3D a whole layer is needed because oblique waves have different normal phase speeds, so a single resistor cannot do the job.

3.2.2 Implementation in the Yee-scheme

Can use the ADE approach, see Dispersive Materials, above

$$\varepsilon j\omega(1+\frac{\sigma}{\varepsilon j\omega})E_z = \partial_y H_x - \partial_x H_y : \quad \varepsilon\partial_t D = \partial_y H_x - \partial_x H_y, \varepsilon\partial_t D = \varepsilon\partial_t E_z + \sigma E$$

$$\mu j\omega(1+\frac{\sigma}{\varepsilon j\omega})^{-1}H_x = \partial_y E_z : \qquad \mu\partial_t K = \partial_y E_z, \varepsilon\partial_t H_x = \varepsilon\partial_t K + \sigma K$$

$$\mu j\omega(1+\frac{\sigma}{\varepsilon j\omega})H_y = -\partial_x E_z : \qquad \mu\partial_t M = -\partial_x E_z, \varepsilon\partial_t M = \varepsilon\partial_t H_y + \sigma H_y$$

where D and E_z, K and H_x, and M and H_y share grid-points, and (E,D) are at integer multiples of Δt and (K,H_x,M,H_y) are at odd half-integer multiples. There result three 2x2 linear systems for (D,E), (K,H_x) and (M,H_y) at the next time level.

3.2.3 Amount of damping; choice of σ.

From the construction, the wave number κ_x is complex,

$$\kappa_x = k_x\mu_2 = k_x(1+\frac{\sigma}{j\omega\varepsilon}), \kappa_y = k_y :$$

$$|E_z(x,y)| = e^{\frac{k_x\sigma x}{\omega\varepsilon}} = e^{-\sigma x/Z\cos\phi} \text{ (remember, Re } k_x < 0)$$

$$\ln\left|E(L)\big/E(0)\right| = -\frac{\sigma L}{Z}\cos\phi$$

for in-coming waves making angle ϕ with the positive x-axis. Since the UPML is terminated by a reflective PEC condition, the reflected wave is also damped, and the net reflection coefficient is

$$\ln|R| = -2\frac{\sigma L}{Z}\cos\phi$$

which can be made as small as we please by choice of σ.

Notes

- Glancing waves ($\phi = \pi/2$) are not damped.
- The damping is independent of wave-length
- Large σ needs special time-stepping for stability reasons (see below)

Because of dispersion, the layer is not completely reflection-free for the Yee discretization. The standard recipe is to increase the damping gradually, like

$$\sigma(x_m) = A(m-n)^p$$

for a layer starting at cell number *m*. The exponent *p* is often chosen $2 < p < 4$. The reflection coefficient over n_{UPML} cells is then

$$\ln|R| = -2\frac{A}{(p+1)Z}(\Delta x \cdot n_{UPML})^{p+1} \cdot \cos\phi$$

3.2.4 Exponential time-stepping

With large σ, the standard central difference time-stepping produces slowly damped oscillations:

$$E^{n+1} = \alpha E^n + \frac{\Delta t/\varepsilon}{1+\beta}\nabla\times H^{n+1/2}, \alpha = \frac{1-\beta}{1+\beta}, \beta = \frac{\sigma\Delta t}{2\varepsilon}$$

Of course, $c\Delta t/\Delta x < 1$ for stability, but if $\beta > 1$, $\alpha < 0$ and there may be wiggles of the $(-1)^n$ kind. This is NOT instability, because the solution still decays, but it is very inaccurate. The problem is that the time-scale of the damping is faster than the transport time scale.

If $\beta < 1$ is restrictive, one may employ "exponentially fitted" time-stepping as follows.

Set $E = Fe^{-\frac{\sigma}{\varepsilon}t}$ and apply the Yee scheme to the equation for *F*:

$$\partial_t F = e^{\frac{\sigma}{\varepsilon}t}\frac{1}{\varepsilon}\nabla\times H : \frac{1}{\Delta t}(e^{\frac{\sigma\Delta t}{\varepsilon}}E^{n+1} - 1\cdot E^n) = e^{\frac{\sigma}{2\varepsilon}\Delta t}\frac{1}{\varepsilon}\nabla\times H^{n+1/2}$$

$$E^{n+1} = e^{-\frac{\sigma\Delta t}{\varepsilon}}E^n + e^{-\frac{\sigma}{2\varepsilon}\Delta t}\frac{\Delta t}{\varepsilon}\nabla\times H^{n+1/2}$$

which is much better for large σ/ε. The standard Yee-formulas can be recovered as rational approximations of degree (1,1) to the exponential functions,

$$e^{-x} = \frac{1-x/2}{1+x/2} + O(x^3) : e^{-\frac{\sigma\Delta t}{\varepsilon}} \approx \frac{1-\beta}{1+\beta}, \beta = \frac{\sigma\Delta t}{2\varepsilon}$$