Contents

1 Mathematics of the Maxwell equations

References:

1. J.D.Jackson, *Classical Electrodynamics*, John Wiley & Sons, 1962 (or later)
2. A.Taflove, S.C.Hagness, *Computational Electrodynamics, the FDTD Method* (2nd. ed.), Artech House, 2000, isbn 1-58053-076-1
3. ("The Book") A.Bondeson, T.Rylander, P.Ingelström ,*Computational Electromagnetics*, Texts in Applied Mathematics 51, Springer, 2005, isbn 0-387-26158-3

This is available as e-book for online reading by KTH students at the link

http://link.springer.com.focus.lib.kth.se/book/10.1007/b136922/page/1

J.C.Maxwell, 1867:

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} + \mathbf{J}_m = 0; \nabla \cdot \mathbf{B} = 0$$

$$\frac{\partial \mathbf{D}}{\partial t} - \nabla \times \mathbf{H} + \mathbf{J}_e = 0; \nabla \cdot \mathbf{D} = \rho$$

$$\mathbf{D} = \varepsilon \mathbf{E}, \mathbf{B} = \mu \mathbf{H}$$

	Electric	Magnetic
Field	**E**, V/m	**H**, A/m
Flux density	**D**, C/m^2	**B**, Wb/m^2
Material	ε, Permittivity	μ, Permeability
Current density	$\mathbf{J}_e$ A/m^2	$\mathbf{J}_m$, V/m^2

For simple materials $\rho \mathbf{J}_e = \mathbf{E}$ and $\rho' \mathbf{J}_m = \mathbf{H}$ with ρ electric (Ohmic) resistivity, $\sigma = 1/\rho$ with σ conductivity and ρ' magnetic resistivity.

- Non-relativistic
- Non-quantized
- Simple material behavior assumed: Cf. ferro-magnetics: hysteresis, etc.

Static (electrostatics, magnetostatics) and quasi-static (induction) behavior was studied before Maxwell, who introduced the displacement current term $d\mathbf{D}/dt$ which gives rise to the electromagnetic waves. The Maxwell equations are the PDE formulation. The equations are hyperbolic and have wave-like solutions. For ε, μ constant and no currents or space charges we obtain by taking the curl and noting

$$\text{div } \mathbf{D} = \text{div } \mathbf{B} = 0,$$

that for any field component *u*,

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{\varepsilon \mu} \Delta u$$

i.e. the wave equation with wave speed $c = \frac{1}{\sqrt{\varepsilon \mu}}$ = speed of light.

Numerical solution of the Maxwell equations as stated above is now a highly developed modeling technique as exemplified in e.g. [2, Ch.1].

When material properties are independent of field amplitudes one often studies time-harmonic solutions – the frequency domain analysis. For cases with piecewise constant ε, μ and currents only on interface surfaces it is possible to formulate surface integral equations for the currents. Numerical solution of properly chosen field integral equations requires discretization of only the surfaces, an order of magnitude fewer degrees of freedom than required for FDTD.

When the size of the domain, measured in wavelengths, is large, numerical resolution of the wavelength becomes very costly. Different approximate methods for short-wavelength computations have been devised. In the zero wavelength limit, wave solutions may be obtained by tracing wavefront normals or rays), the geometrical optics approximation. But many simulations must include diffraction phenomena, and corrections to the geometrical optics such as the Uniform theory of diffraction have been developed, starting with Keller's work in the sixties on diffraction coefficients.

Numerics taxonomy
TD = time domain, FD = Frequency domain
FD = Finite Difference, FV = Finite Volume, FE = Finite Element, MoM = Method of Moments

	Time domain	**Frequency domain**
PDE	*FDTD (Yee, 1966)* FVTD e.g. Shang FETD Bondesson	FEFD (many)
Integral	Chew, Illinois (1998?)	*MoM (Harrington 1968)* *Rao, Glisson, Wilson* Nedelec, Monk, …
Rays	-??	Keller – only overview

1.1 First order linear systems of partial differential equations with a time-like variable

First order system of *N* PDE with *t* as time-like variable, *n* space dimensions:

$$\frac{\partial \mathbf{u}}{\partial t}+\sum_{k=1}^{n}\mathbf{A}_k\frac{\partial \mathbf{u}}{\partial x_k}=0,\mathbf{u}(\mathbf{x},t)\in\Re^N$$

Wave-like solution

$$\mathbf{u}(x,t)=\mathbf{a}(x,t)e^{iS(x,t)},\mathbf{a}:\text{amplitude},S:\text{phase.}$$

An iso-surface, locus of points of equal phase, *S* = *const.* is a wavefront. Constant coefficients $\mathbf{A}_k$ allow **a** = constant vector. Then

$$(S_t\mathbf{I}+\sum\mathbf{A}_iS_{x_i})\mathbf{a}=0;\lambda=\frac{S_t}{\sqrt{\sum\left(S_{x_i}\right)^2}}\Rightarrow$$

$$(\lambda\mathbf{I}+\sum\mathbf{A}_i\gamma_i)\mathbf{a}=0,\gamma_i=\frac{S_{x_i}}{\sqrt{\sum\left(S_{x_i}\right)^2}}=\cos\phi_i$$

Hyperbolic, if $\sum\mathbf{A}_i\gamma_i$ has a complete set of eigenvectors and real eigenvalues $\{\lambda_i\}$

Non-trivial solutions: **a** must be an eigenvector and $-\lambda$ the corresponding eigenvalue
Normal to surface is $(\gamma_1,\gamma_2,..,\gamma_n,\lambda)$.

The front moves in its normal direction with phase-speed $-\lambda$.

For $dS = S_t dt + \sum dx_i S_{x_i} = 0$. Take $dx_i = \gamma_i\, \delta$, a small displacement in normal direction.

Then $S_t dt + \delta\sqrt{\sum \left(S_{x_i}\right)^2} = 0$ and $\dfrac{\delta}{dt} = -\lambda$

Note
• λ may depend on the wave normal direction. If not, isotropic.
• *N* different waves **a**

Let us look at the Maxwell equations in this framework, a pure initial value problem for all of empty space $\mathcal{R}^3$, to simplify matters take ε = μ = 1 (no restriction). The matrices become (cf. the curl formula)

$$\mathbf{A}_i = \begin{pmatrix} 0 & \mathbf{G}_i^T \\ \mathbf{G}_i & 0 \end{pmatrix}, \mathbf{G}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \mathbf{G}_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \mathbf{G}_3 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

This shows why the signs of curl in the two equations differ: that makes the system symmetric, because curl in itself is an "anti-selfadjoint" operator. So

$$\sum \gamma_i \mathbf{A}_i = \begin{pmatrix} 0 & \mathbf{G}^T \\ \mathbf{G} & 0 \end{pmatrix} \text{ with } \mathbf{G} = \begin{pmatrix} 0 & \gamma_3 & -\gamma_2 \\ -\gamma_3 & 0 & \gamma_1 \\ \gamma_2 & -\gamma_1 & 0 \end{pmatrix}.$$

and the eigensystem satisfies

$$\begin{pmatrix} 0 & \mathbf{G}^T \\ \mathbf{G} & 0 \end{pmatrix}\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \text{ or } \mathbf{G}^T\mathbf{G}\mathbf{x} = \begin{pmatrix} \gamma_3^2+\gamma_2^2 & -\gamma_1\gamma_2 & -\gamma_1\gamma_3 \\ -\gamma_1\gamma_2 & \gamma_1^2+\gamma_3^2 & -\gamma_2\gamma_3 \\ -\gamma_1\gamma_3 & -\gamma_2\gamma_3 & \gamma_1^2+\gamma_2^2 \end{pmatrix} = \lambda^2\mathbf{x};$$

$\mathbf{G}^T\mathbf{G} = \underbrace{|\gamma|^2}_{=1} - \gamma\gamma^T$ has an eigenvalue 0 with eigenvector **γ**, and two eigenvalues 1 whose invariant subspace is the set of all vectors normal to **γ**. Thus, for the 6x6 $\sum \mathbf{A}_k\gamma_k$ matrix there are two static fields (the zero eigenvalues) and four waves moving "left and right" with velocity 1 – remember μ = ε = 1. These are *transversal waves*: the eigenvectors are orthogonal to **γ**, the wavefront normal.

Example – Exercise 1
Waves moving in the (*x*,*y*)-plane, H-field **H** = (0,0,*H*),

$$\varepsilon\frac{\partial E_x}{\partial t} = \frac{\partial H}{\partial y}; \varepsilon\frac{\partial E_y}{\partial t} = -\frac{\partial H}{\partial x}; \mu\frac{\partial H}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}$$

$$\mathbf{u} = \begin{pmatrix} E_x \\ E_y \\ H \end{pmatrix} : \mathbf{u}_t + \mathbf{A}_1\mathbf{u}_x + \mathbf{A}_2\mathbf{u}_y = 0,$$

Write the matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ and compute the eigenvalues and eigenvectors of cos ϕ $\mathbf{A}_1$ + sin ϕ $\mathbf{A}_2$ to conclude that

i) wave speed (of light) $c = \dfrac{1}{\sqrt{\varepsilon\mu}}$ independent of direction, isotropic

ii) the **E** and H fields, for the traveling waves, are transversal, i.e. orthogonal to the direction of travel.

1.2 Energy estimates.

The wave solutions above neither grow nor decay with time. That this is true for any solution can be easily shown, again using the symmetry of the curl equations.

$$\left.\begin{aligned}\mu\mathbf{H}_t+\nabla\times\mathbf{E}=0\\ \varepsilon\mathbf{E}_t-\nabla\times\mathbf{H}=0\end{aligned}\right\}\Rightarrow \underbrace{\mu\mathbf{H}}_{\mathbf{B}}\cdot\mathbf{H}_t+\underbrace{\varepsilon\mathbf{E}}_{\mathbf{D}}\cdot\mathbf{E}_t+\mathbf{H}\cdot(\nabla\times\mathbf{E})-\mathbf{E}\cdot(\nabla\times\mathbf{H})=0,$$

$$\frac{1}{2}\frac{\partial}{\partial t}\left(\int_{R^3}\left(\mu\mathbf{H}\cdot\mathbf{H}+\varepsilon\mathbf{E}\cdot\mathbf{E}\right)dV\right)+\underbrace{\int_{R^3}\left(\mathbf{H}\cdot(\nabla\times\mathbf{E})-\mathbf{E}\cdot(\nabla\times\mathbf{H})\right)dV}_{=0***)}=0$$

$$\text{or}:\ \mu\left\|\mathbf{H}(.,t)\right\|_2^2+\varepsilon\left\|\mathbf{E}(.,t)\right\|_2^2=const.=\mu\left\|\mathbf{H}(.,0)\right\|_2^2+\varepsilon\left\|\mathbf{E}(.,0)\right\|_2^2$$

Example: Show that the integral ***) vanishes whenever **E** and **H** vanish at infinity. Hint: Integration by parts.

This proves that the "energy" is conserved. This is more generally true, e.g. also in the presence of perfectly reflecting surfaces. However, other measures of the solution may grow: A mirror can focus the waves so that the maximal field (the L_∞ norm) becomes essentially unbounded.

2 Basics of Difference Schemes for Wave Problems

References:
H-O.Kreiss, B.Gustafsson, J.Oliger: *Time Dependent Problems and Difference Methods*, John Wiley & Sons, 1996

The scheme to be presented in detail is the Yee, or staggered grid Leap-frog, scheme which has a number of advantages. In order to better appreciate Yee, we will introduce analysis tools, which display important properties of schemes, and apply them to other (very simple) schemes.

Consider first difference schemes for pure initial value problems in 1D plus time.

Derivatives replaced by difference quotients, for example

$$\left.\frac{\partial f}{\partial x}\right|_{x,t}=\frac{f(x+\Delta x,t)-f(x,t)}{\Delta x}+O(\Delta x^p).\ p=\text{order of accuracy}=1:\text{Forward difference.}$$

$$\left.\frac{\partial f}{\partial x}\right|_{x,t}=\frac{f(x+\Delta x,t)-f(x-\Delta x,t)}{2\Delta x}+O(\Delta t^2).\ \text{Central difference.}$$

$$\text{Grid}:\left\{(x_j,t_n)\right\}_{j,n=0,1,2,\ldots}.x_j=j\Delta x,t_n=n\Delta t.u_j^n\approx u(x_j,t_n)$$

Concepts:
Convergence, consistency, well-posedness, growth of solutions, stability,

A necessary property is *convergence*, which means that for a fixed *t* and *x*, as Δt and Δx -> 0 (such that there always is a u_j^n at exactly the right spot) $u_{j(\Delta x)}^{n(\Delta t)}\to u(x,t)$.

Consistency means that when u_j^n are chosen as samples of a smooth function *u*(*x*,*t*), the difference scheme formally converges to the differential equation. The analysis is done by substituting Taylor expansions and cancelling terms. This operation is mechanical and difference operator calculus can be used to simplify the actual manipulations.

Well-posedness is a mathematical characterization of a problem, which requires

- existence of a "locally unique" solution
- that the solution be continuous as function of the problem parameters, such as initial data

For initial value problems, well-posedness is equivalent to *bounded growth*:
The homogeneous problem with initial value $u(x,0) = f(x)$ is well-posed if and only if there exist constants K and α, independent of f, such that

$$\|u(.,t)\| \le Ke^{\alpha t}\|f\|,$$

The numerical counterpart to well-posedness is *stability*, which roughly speaking for initial value problems means bounded growth of perturbations in the discrete scheme.
Let the numerical solution at time t_n be $\mathbf{u}_n = (\ldots, u_{j-1}^n, u_j^n, u_{j+1}^n, \ldots)$, then the scheme applied to the equation is called stable if and only if there exists a b independent of n, f and Δx, Δt such that

$$\|\mathbf{u}^{n+1}\|/\|\mathbf{u}^n\| \le 1 + b\Delta t$$

As a test problem we take hyperbolic constant coefficient linear systems,

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{u}}{\partial x} = 0 \qquad (2.1)$$

Example
The second order wave equation can be written as a first order system,

$$\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2} \Rightarrow \begin{cases} \frac{\partial u}{\partial t} + c\frac{\partial v}{\partial x} = 0 \\ \frac{\partial v}{\partial t} + c\frac{\partial u}{\partial x} = 0 \end{cases}, \mathbf{A} = \begin{pmatrix} 0 & c \\ c & 0 \end{pmatrix}$$

(General theoretical analysis of Boundary conditions is outside the scope of this course.)
The system is assumed hyperbolic and can be diagonalized by exchanging the primitive variables **u** for the characteristic variables **w**, related by

$$\mathbf{u} = \mathbf{V}\mathbf{w}$$

where **V** is the matrix of (right) eigenvectors of **A**. The system becomes

$$\frac{\partial \mathbf{w}}{\partial t} + \Lambda\frac{\partial \mathbf{w}}{\partial x} = 0\,,\ \Lambda = \mathrm{diag}(\lambda_1, \lambda_2, ..., \lambda_N) \ \text{ or } \frac{\partial w_k}{\partial t} + \lambda_k\frac{\partial w_k}{\partial x} = 0, k = 1,2,...,N$$

For any linear scheme, the operations of discretization and diagonalization commute, so it is clear that we can restrict our study to the single equation

$$u_t + au_x = 0$$

to which we apply the simplest, first order accurate in time and space scheme:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^n - u_j^n}{\Delta x} = 0, \text{ or } u_j^{n+1} = (1+\sigma)u_j^n - \sigma u_{j+1}^n$$

where $\sigma = a\Delta t/\Delta x$ is called the Courant (sometimes the Courant-Friedrichs-Lewy) number which tells how many cells the wave travels in a timestep.

2.1 Fourier (or Von Neumann) analysis

The difference formulas, just as the differential equations, allow exponentials as solutions and we look for a solution with wave number k ($= 2\pi/\lambda$, λ = wavelength):

$$u_j^n = G^n e^{ikx_j}$$

G is called the growth factor; if $|G| > 1$ the wave grows and $|G| < 1$ means a damped wave.
If G is real, the phase depends on x only: a standing wave, no propagation.

Note: One need not diagonalize the system for the stability analysis. For a system of *s* equations, **G** becomes an *s* x *s* matrix.
By substituting the ansatz, we obtain

$$G = (1+\sigma) - \sigma e^{ik\Delta x} = 1 + \sigma\left(1 - \cos\theta - i\sin\theta\right)$$

where $\theta = k\Delta x$ = phase shift per cell. The relevant range for θ is $-\pi$ to π; a wave with shorter wavelength is indistinguishable ***on the grid*** from one with wavelength in this range. Think of the Shannon sampling theorem.
The growth factor for the exact solution is

$H = \exp(-iak\Delta t) = \exp(-i\sigma\theta)$. Its phase speed is of course

$a = -(\arg H)/(k\Delta t)$. Similarly, the phase speed of the numerical solution is

$a_n = -(\arg G)/(k\Delta t)$

The further analysis requires an assumption of how Δt and Δx tend to 0; the usual assumption is that σ is kept constant. We have

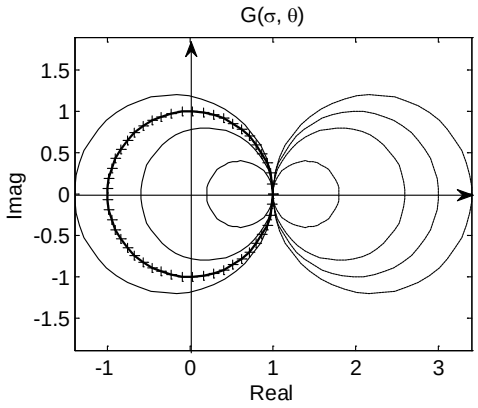
$$G = 1 + \sigma(\theta^2/2 - i(\theta - \theta^3/6)) + O(\theta^4)$$

$$H = 1 - i\sigma\theta - \sigma^2\theta^2/2 + \ldots$$

So, arg H = arg G to first order in θ, i.e. Δx and Δt, and

$a_n = a + O(\Delta t)$ as $\Delta t \to 0$, for a fixed Courant number.

For finite step-sizes, the phase speed depends on the wavelength. This is called *dispersion*.
It is clear that $|H| = 1$ cf. the L2 norm analysis for the Maxwell equations, the energy is conserved. But $|G|$ depends on σ and θ. $|G| < 1$ is *dissipation* (damping), $|G| > 1$ is growth.



Here is a plot of the locus of $G(\theta,\sigma)$ in the complex plane for σ=-1.2,-1,-0.8,-0.4,(solid) 0.4,0.8,1, and 1.2 (dashed), $-\pi \le \theta \le \pi$. The unit circle is marked by +. For σ = -1, the scheme has $|G| = 1$, for $-1 < \sigma < 0$ it is damped, $|G| < 1$: $\sigma = 0$ is uninteresting and for other σ it is unstable.

Turning the space difference the other way we get

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_j^n - u_{j-1}^n}{\Delta x} = 0, \text{ or } u_j^{n+1} = (1-\sigma)u_j^n + \sigma u_{j-1}^n$$

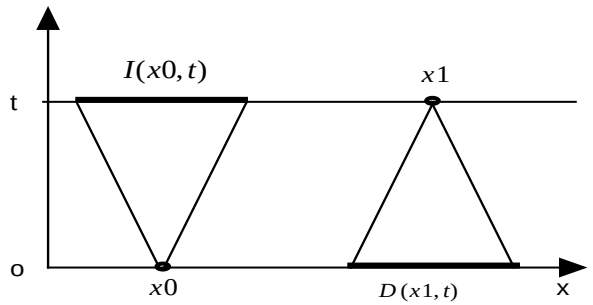
which is damped for $0 < \sigma < 1$ and unstable for other σ. It appears that the difference scheme should be chosen to reflect the direction of the characteristics: *upwind* or *upstream* differencing is useful. Why this is so can be illustrated by the

2.2 Courant-Friedrichs-Lewy sufficient condition for non-convergence.

Concepts: domain of dependence, domain of influence.
Consider again an initial value problem for a system of PDE in time and one space dimension, initial values $\boldsymbol{u}(x,0) = \boldsymbol{f}(x)$. The domain of dependence is the sub-set $D(x,t)$ of the x-axis such that $\boldsymbol{f}(x)$ for x outside D has no influence on $\boldsymbol{u}(x,t)$. For hyperbolic systems, a plot of the characteristics through (x^*,t^*) immediately reveals D: it is the section cut off by the extreme characteristics

$x - x^* = \max(\lambda_j)(t - t^*)$ and $x - x^* = \min(\lambda_j)(t - t^*)$.

That D is bounded is referred to as finite speed propagation of information. For the heat equation, D is all of space $(-\infty,\infty)$ and information travels infinitely fast, although distant points influence the solution less than near-by points. The domain of influence is the reverse: The set $I(x^*,t)$ for which $\boldsymbol{f}(x^*)$ influences $\boldsymbol{u}(x,t)$. See the figure. For the numerical scheme the definition is analogous.

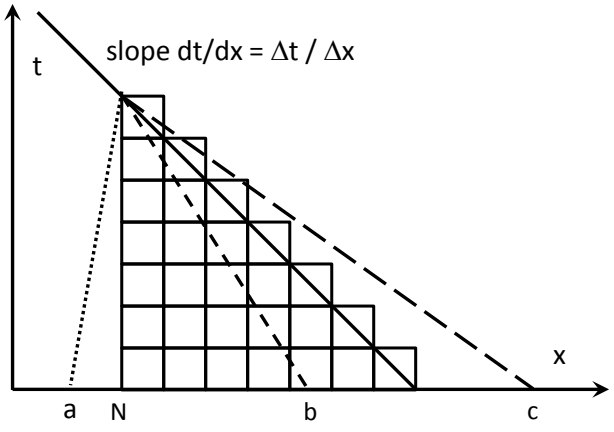


Domain of dependence *D* and Influence *I* for second-order wave equation

$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0$. The slopes are $dt/dx = \pm 1/c$.

It is now clear that for convergence to be possible, the numerical domain of dependence *N* must include the mathematical domain of dependence *D*: This is the CFL condition which is necessary for convergence. If it does not hold, we can change the exact solution at will by manipulating ***f***(*x*) for *x* outside *N* but in *D*, i.e., without changing the numerical solution.
The *Lax Equivalence Principle* shows that what happens is numerical instability:
The principle says - again, roughly, but with the proper preparations this is a theorem -

convergence = stability & consistency



So for a consistent scheme (which all of the schemes considered here are, and it is easy to check) it is only stability that can go wrong. Hence, violation of the CFL-condition implies instability. The CFL condition is easy to picture by overlaying the computational grid on the domain of dependence. For the first single sided scheme above the picture is:
a shows a case with $a(\sigma) > 0$, unstable because the difference scheme looks the wrong way, *b* is a (possibly) stable case, and *c* again is unstable because the timestep is too large. The plots of *G* confirm that *b* is actually stable. The final stability condition for the single-sided scheme is

$-1 < \sigma < 0$

and with the difference turned the other way,

$0 < \sigma < 1$

The following scheme (Lax-Friedrichs) is symmetric and avoids the necessity to switch directions:

$$\frac{u_j^{n+1} - u^*}{\Delta t} + a\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = 0, \text{ where } u^* = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right)$$

As is easily seen, the CFL condition is $|\sigma| < 1$ and this is also a sufficient condition as may be shown by the Fourier analysis. It is left as homework to experiment with the scheme and look at its dissipation and dispersive properties.
Note: This scheme is ***never*** used for the Maxwell or simple wave equations because of its excessive damping. It can be used as a starting point for more accurate schemes for nonlinear problems, such as in gas dynamics, where dissipation is absolutely necessary to control shock formation etc.

2.3 Finite differences for wave equations

(Book pp 27-33)

The *approximation properties* of difference approximation to derivatives are characterized by the order of accuracy *p*, and the error coefficient *C*; Let the grid be $\{x_i\}$, $x_i - x_i = h$ (equidistant, meshsize *h*) and approximate the derivative $f'(x_i)$ for a smooth function *f* by some difference formula

$$(Lf)(x_i) = \frac{1}{h}\sum_{k=-s}^{s} \alpha_k f(x_{i+k})$$

The error is then

$$e = f'(x_i) - (Lf)(x_i) = Ch^p f^{(p+1)}(x_i) + o\left(h^{p+1}\right)$$

Examples

$$f'(x_i) - \underbrace{\frac{1}{h}(f_{i+1} - f_i)}_{D_+ f_i} = \frac{1}{2}hf'' + o(h^2) \qquad \text{Forward}$$

$$f'(x_i) - \underbrace{\frac{1}{h}(f_i - f_{i-1})}_{D_- f_i} = -\frac{1}{2}hf'' + o(h^2) \qquad \text{Backward}$$

$$f'(x_i) - \underbrace{\frac{1}{2h}(f_{i+1} - f_{i-1})}_{D_0 f_i} = \frac{1}{6}h^2 f^{(3)} + o(h^4) \qquad \text{Central}$$

$$\left.\begin{aligned} f'(x_i) - \frac{1}{h}(f_{i+1/2} - f_{i-1/2}) &= \frac{1}{24}h^2 f^{(3)} + o(h^4) \\ f'(x_{i+1/2}) - \frac{1}{h}(f_{i+1} - f_i) &= \frac{1}{24}h^2 f^{(3)} + o(h^4) \end{aligned}\right\} \text{Central on staggered grid}$$

The two "different" staggered grid formulas differ only by numbering of points; if values of *f* are available on the grid, we obtain values for the derivative at $x_{i+1/2}$ (midway between neighbor points) with step *h*, and at points x_i with step 2*h* (the D_0 formula).

But there is more than approximation to solving differential equations. We replace them by difference equations to obtain approximations u_i to the solution (say $u(x)$) at the gridpoints, so the error is

$$e_i = u(x_i) - u_i$$

Example

Central differences for second order "Helmholtz" equation

In contrast to the schemes discussed above, this is an extremely successful scheme. For a time-harmonic solution $v(x,t) = e^{i\omega t}u(x)$ to the wave equation $v_{tt} = c^2 v_{xx}$, with wave number $k = \omega/c$ it gives (think of periodic boundary conditions, or a Cauchy-problem)

$$u'' + k^2 u = 0 : u_{m+1} - 2u_m + u_{m-1} + h^2 k^2 u_m = 0$$

Characteristic equation : $G^2 - (2 - \theta^2)G + 1 = 0$

$$G_{1,2} = 1 - \frac{\theta^2}{2} \pm \left(\theta^4/4 - \theta^2\right)^{1/2} = 1 - \frac{\theta^2}{2} \pm i\theta\left(1 - \theta^2/4\right)^{1/2}$$

$$= 1 \pm i\theta - \frac{\theta^2}{2} + O(\theta^3) = e^{\pm i\theta} + O(\theta^3)$$

The exact solution is $Ae^{ikx} + Be^{-ikx} = C\cos kx + D\sin kx$. Subject to the (stability) stepsize requirement $|kh| \le 2$, the numerical solutions are of the exactly the same form but with slightly modified wave numbers,

$$h \cdot k_{num} = \arccos\left(1 - \frac{k^2 h^2}{2}\right) \Rightarrow k_{num} = k \cdot \left(1 + O(k^2 h^2)\right)$$

Violation of the stepsize limit gives catastrophic growth of error in attempts to propagate the wave.

3 FDTD

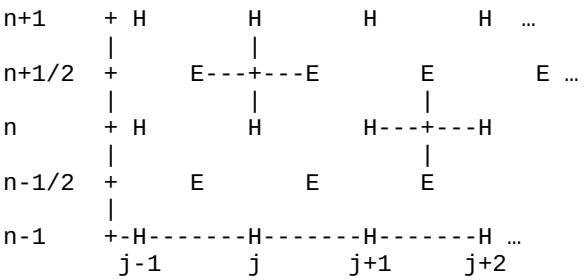
Book Ch 5: FDTD

FD = finite difference, TD = time domain

"FDTD" is now used to mean specifically the scheme popularized by Kane S. Yee in 1966, with a grid staggered in time and space. This allows centered differences for all variables, in time and space. We look first at the staggered grid scheme for 1D Maxwell w/o dissipation (lossless material)

$$\varepsilon E_t = H_x, \mu H_t = E_x$$

Grid: Vertical time, horizontal *x*. Usually time index set as superscript, space index as subscript.



Update formulas:

$$H_j^{n+1} - H_j^n = \frac{\Delta t}{\mu \Delta x}(E_{j+1/2}^{n+1/2} - E_{j-1/2}^{n+1/2})$$

$$E_{j+1/2}^{n+1/2} - E_{j+1/2}^{n-1/2} = \frac{\Delta t}{\varepsilon \Delta x}(H_{j+1}^n - H_j^n)$$

This first order system of difference equations is equivalent to

$$u_j^{n+1} - 2u_j^{n+1} + u_j^{n+1} = \sigma^2(u_{j+1}^n - 2u_j^n + u_{j-1}^n), \sigma = \frac{c\Delta t}{\Delta x}$$

where *u* can be *E* or *H*, just like either of $E(x,t)$ and $H(x,t)$ satisfy the wave equation

$$u_{tt} = c^2 u_{xx}, c^2 = \frac{1}{\varepsilon \mu}$$

σ is called the Courant number, the ratio between the distance traveled by the wave in a timestep and the cell size.

3.1 Dispersion: Phase speed depends on wavelength

The discretized equation has wave-solutions $u_j^n = U_n e^{ikx_j}$ - because exponential functions are eigenfunctions of constant coefficient difference as well as differential operators. Substitute the ansatz in the difference equation,

$$(U_{n+1} - 2U_n + U_{n-1})e^{ikx_j} = \sigma^2 U_n (e^{ik(x_j+\Delta x)} - 2e^{ikx_j} + e^{ik(x_j-\Delta x)})$$

$$U_{n+1} - 2U_n + U_{n-1} = \sigma^2 U_n (e^{ik\Delta x} - 2 + e^{-ikx}) = -4\sigma^2 U_n \sin^2\frac{\theta}{2}, \theta = k\Delta x$$

This difference equation has solutions of type $U_n = \xi^n$ where ξ satisfies the characteristic equation

$$\xi - (2 - 4\sigma^2 \sin^2\frac{\theta}{2}) + \xi^{-1} = 0$$

The general solution is $U_n = a\xi_1^n + b\xi_2^n$ where ξ_i are the roots of the characteristic equation. For this wave NOT to grow, the moduli of ξ_1 and ξ_2 must be <= 1. But the product of roots is 1, so in that case both roots have modulus 1, $\xi_1 = \exp(i\alpha)$, $\xi_2 = \exp(-i\alpha)$ and

$$\cos\alpha = 1 - 2\sigma^2 \sin^2\frac{\theta}{2}$$

or

$$\sin\frac{\alpha}{2} = \pm\sigma \sin\frac{\theta}{2}$$

which is possible (with real α) if $\sigma^2 \sin^2\frac{\theta}{2} \le 1$ for all wave numbers θ, i.e., $\sigma <= 1$.

Now, this means that the wave phase changes by α per timestep Δt,

$$u_j^n = e^{i(\frac{\alpha t}{\Delta t} + kx_j)} = e^{i(\omega t + kx_j)}$$

so the phase speed of the wave is

$$c_{num} = \omega/k = \alpha/(k\Delta t) = \alpha c/(\sigma\theta)$$

or

$$c_{num}/c = \alpha/(\sigma\theta)$$

We see that the wave speed depends on

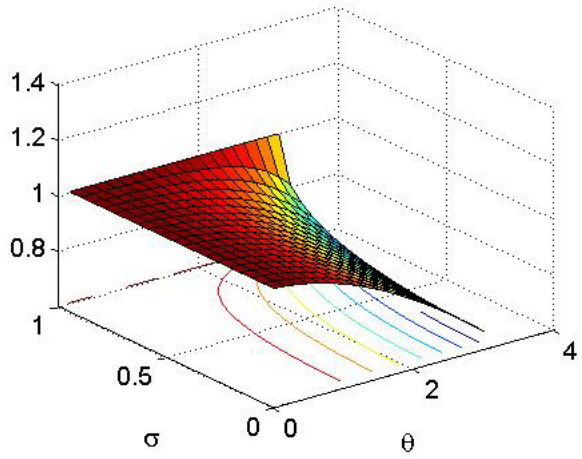
spatial resolution: $2\pi/\theta$ is the number of cells per wavelength.

temporal resolution: σ is the number of cells traveled in a timestep

and this *dispersion* is the most important error in the solution. The waves are NOT *dissipative* because the amplitude is constant: $|\xi| = 1$ when the time-step is limited to $\sigma <= 1$.

The plot shows c_{num}/c as function of σ and θ.

- The error vanishes as θ -> 0: the scheme converges for any stable σ.
- It is correct *independent* of θ if σ = 1: The magic time-step.
- The error seems never worse than 40% and the wave always is too slow;
- Short waves (larger θ) run more slowly that longer.



The error in phase speed could be fixed for monochromatic waves by modifying the material data

so the numerical speed matches the desired, but the Magic time-step is not possible anyway in 2 & 3D for stability reasons.

3.1.1 Anisotropy and stability

In 2D and 3D the numerical wave speed varies also with the direction of the wave. Consider the 2D case; the Yee scheme is equivalent to the central difference discretization of the wave equation, and assuming the wave travels with a wavefront normal (cos ϕ, sin ϕ) we obtain after a manipulation much like the 1D above that the phase shift per time step α satisfies

$$\sin^2\frac{\alpha}{2}=\sigma^2\left(\sin^2\frac{\theta\cos\phi}{2}+\sin^2\frac{\theta\sin\phi}{2}\right)$$

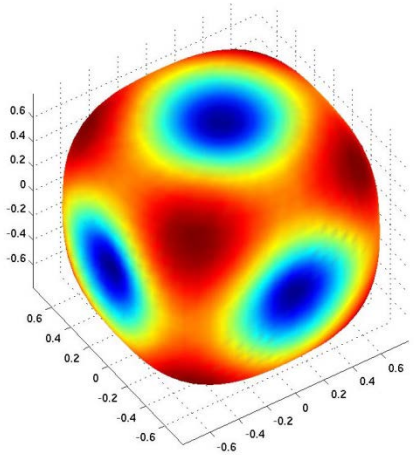
and for 3D

$$\sin^2\frac{\alpha}{2}=\sigma^2\left(\sin^2\frac{\theta\cos\phi_1}{2}+\sin^2\frac{\theta\cos\phi_2}{2}+\sin^2\frac{\theta\cos\phi_3}{2}\right)$$

where the $\cos\phi_k$ are the direction cosines of the wavefront normal. There must be a real α for all wavenumbers θ, and all wave directions, so the max. over ϕ and θ of the RHS must not exceed 1. Thus, the time step is limited to

$$\frac{c\Delta t}{\Delta x}\le\frac{1}{\sqrt{D}}$$

in D space dimensions, assuming equal mesh increments in all dimensions. The waves travel fastest along the main diagonals, and most slowly along the grid lines.



The colored die is a representation of the anisotropy in a 3D FDTD model. The wave speeds depend on the wave direction. A point on the die represents the corresponding propagation direction, its distance to the origin (and its color) shows the wave speed c_{num}/c, with 12 cells per wavelength and a CFL-number of 0.99/sqrt(3). The shape is exaggerated: $0.9923 < c_{num}/c < 0.9999$, so a difference of less than one %.

3.2 Complexity and error

Armed with a formula for the dispersion error we can estimate the work for solving a diffraction problem over a domain of size L (L^2 in 2D, L^3 in 3D).
Suppose a phase error of E (compared to the exact solution) is acceptable. The waves travel L and have wavelength λ and accumulate phase error

$$(1-\frac{c_{num}}{c})\frac{L}{\lambda}<E$$

For small θ, we obtain

$$\frac{\alpha}{\sigma\theta}=1-\frac{\theta^2}{6}+O(\theta^4)$$

so it is necessary that

$$E>\frac{L}{\lambda}\frac{\theta^2}{6}=\frac{4\pi^2L}{6\lambda^3}\Delta x^2$$

The number of time-steps to travel L is $n = L/(\sigma\,\Delta x)$ and in D space dimensions there are $(L/\Delta x)^D$ cells so the total work is

$$\frac{1}{\sigma}\left(\frac{L}{\Delta x}\right)^{D+1} W_D > \frac{1}{\sigma}\left(\frac{L\cdot L^{1/2}}{\sqrt{\frac{6E}{4\pi^2}}\lambda^{3/2}}\right)^{D+1} = Const.\frac{\sqrt{D}W_D}{E^{\frac{D+1}{2}}}\left(\frac{L}{\lambda}\right)^{\frac{3(D+1)}{2}}$$

where W_D is the work to for one time step on one cell. In 3D, for example, the work grows as the *sixth power* of the electrical size L/λ and as the inverse square of the phase error accepted. The table below shows the phase error in ^{o} for a range of L/λ and 2^k cells per wavelength, $k = 1\ldots7$, errors of more than 360^o replaced by 360^o. A common recommendation is $O(12)$ cells per wavelength, but as we see, electrically large cases require much more than that.

Table1: Phase error, degrees; N = #cells per wavelength, Size = L/wavelength

N	2	4	8	16	32	64	128	256
Size								
1	74.85	8.68	1.85	0.44	0.11	0.03	0.01	0.00
10	360.00	86.79	18.47	4.45	1.10	0.27	0.07	0.02
100	360.00	360.00	184.72	44.49	11.02	2.75	0.69	0.17
1000	360.00	360.00	360.00	360.00	110.21	27.49	6.87	1.72
10000	360.00	360.00	360.00	360.00	360.00	274.90	68.69	17.17

Table 2, 10log(W)

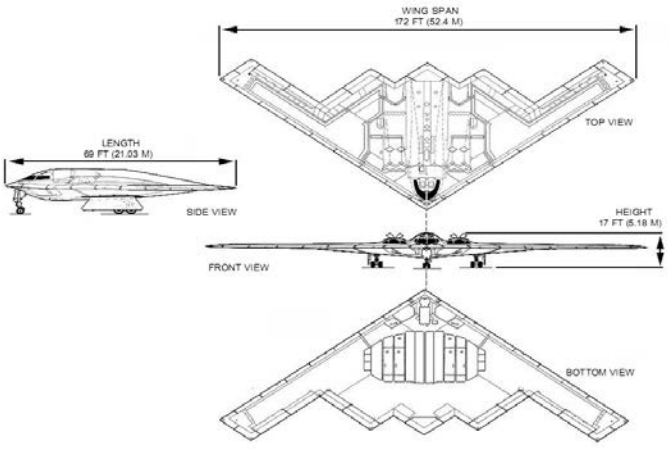
N	2	4	8	16	32	64	128	256
Size								
1	0.90	1.81	2.71	3.61	4.52	5.42	6.32	7.22
10	3.90	4.81	5.71	6.61	7.52	8.42	9.32	10.22
100	6.90	7.81	8.71	9.61	10.52	11.42	12.32	13.22
1000	9.90	10.81	11.71	12.61	13.52	14.42	15.32	16.22
10000	12.90	13.81	14.71	15.61	16.52	17.42	18.32	19.22

Suppose 10^o phase error is acceptable:

Size	1	10	100	1000
N	4	12	32	100
#cells	64	1.7M	33G	1P
10logW	2	6	10	15

(M,G,T,P = Mega,Giga,Tera,Peta = $10^{6,9,12,15}$)

Clearly, for this accuracy requirement, $L/\lambda = 10^3$ is out of reach at present, but L/λ a few 100's is possible on a large computer. $L/\lambda = 10$ is easy on your PC.



The wing-span of a B2 Spirit is 52m and search radars have λ $O(0.1\text{m})$. The craft was designed in the eighties, on machines (like the Cray XMP/48) capable of 100 Mflops with 64 M words memory.
Obviously, other techniques than second order FDTD were used! We shall see later how the integral equation methods would fare. The rectilinear planform is typical of early stealth designs, like the F117 NightHawk, which was made of all flat surfaces.

3.3 Improvements?

Higher order difference formulas are effective for wave propagation, on a regular grid. But the Yee scheme staircase approximations to oblique boundaries would destroy the potential higher accuracy. Also, construction of higher order accurate and stable boundary conditions is not easy.
The most successful attempts are the "summation by parts" operators developed at TDB, Uppsala (Gustafsson, Strand, Nordström & al), and the Embedded Boundary schemes (Leveque, Kreiss, Petersson). Most codes still rely on the second order formulas, and use various types of mesh refinement and/or triangular/tetrahedral meshes close to boundaries to mitigate the staircase effects.

4 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.

4.1 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

$$u_t + c u_x = 0 \text{ (and the right-running: } u_t - c u_x = 0 \text{)}$$

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 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.

4.1.1 Reflection & Engquist-Majda non-reflecting conditions

We have derived a non-reflecting condition by considering 1-D waves and the characteristics. The condition admits only waves traveling with outward velocity *c* (phase speed of light). What happens if we apply it on a multi-dimensional wave problem on a half-space $x < 0$?
Say 2D (x,y).

For $x < 0$, the wave equation $u_{tt} = c^2(u_{xx} + u_{yy})$, on the right half - space $x > 0 : u_t + cu_x = 0$

Time-harmonic variation $u = e^{i\omega t}U(x, y)$, and $k = \omega/c = 2\pi/\lambda$. Let the incoming wave be $U_{inc} = \exp\big(i(k_x x + k_y y)\big)$, the reflected $U_{sc} = R\exp\big(i(\kappa_x x + \kappa_y y)\big)$ and the transmitted wave $U_{tr} = T\exp\big(i(ax + by)\big)$.

$k^2 = k_x^2 + k_y^2$ is the dispersion relation for the left half plane, so it follows that

$\kappa_x{}^2 + \kappa_y{}^2 = k^2$ and likewise, $a^2 + b^2 = k^2$

Indeed, $b = 0$ and $k = a$, for the characteristic condition, but we will keep the generality for the moment. This defines the reflection coefficient *R* and the transmission coefficient *T*. At $x = 0$ the waves on the two half-planes must match,

$U_{inc} + U_{sc} = U_{tr}$, and $\mathrm{d/dx}(U_{inc} + U_{sc}) = \mathrm{d/dx}(U_{tr})$:

$$e^{ik_y y} + Re^{i\kappa_y y} = Te^{iby}, k_x e^{ik_y y} + \kappa_x Re^{i\kappa_y y} = aTe^{iby} \text{ or}$$
$$k_x e^{ik_y y} + \kappa_x Re^{i\kappa_y y} = a\left(e^{ik_y y} + Re^{i\kappa_y y}\right) : e^{ik_y y}(k_x - a) = Re^{i\kappa_y y}(a - \kappa_x)$$

and the reflection coefficient becomes

$$R = \frac{k_x - a}{a - \kappa_x} = \frac{k_x - a}{a + k_x} = \frac{k\cos\theta - a}{k\cos\theta + a}$$

It follows, that $\kappa_y = k_y$ and $\kappa_x = -k_x$ because the scattered wave must move away from the interface. Thus, with the characteristic condition, $a = k$ and

$R = (\cos\theta - 1)/(1 + \cos\theta) = -\tan^2(\theta/2)$

where θ is the angle between interface normal and wavefront normal.
Example: A source in the center of a square sees a maximal θ of 45^o to the corners where *R* becomes $3 - \sqrt{8} = .17$

The Mur first order condition, discretized as shown, gives a small reflection even for orthogonal waves because the numerical wave speed differs slightly (parts of %) from *c*. As we just saw, non-orthogonal waves give much larger reflection, so it makes sense to look for continuous models with smaller reflection. This is the subject of the Engquist–Majda family of conditions. The technique is to derive approximations in wave-number space which are transformed back into physical space by

$i\omega = \mathrm{d/dt}$, $-ik_x = \mathrm{d/dx}$, etc.

The dispersion relation is $k_x{}^2 + k_y{}^2 = k^2$:

$$k_x = \pm\left(k^2 - k_y^2\right)^{1/2} = \pm k\left(1 - \frac{k_y^2}{k^2}\right)^{1/2}$$

$$1st\text{ order}: k_x = -k = -\frac{i\omega}{ic}; -ick_x + i\omega = 0 : cu_x + u_t = 0$$

$$2nd\text{ order}: k_x = -k\left(1-\frac{1}{2}\frac{k_y^2}{k^2}\right); kk_x = \frac{\omega}{c}k_x = -k^2 + \frac{1}{2}k_y^2 = -k_x^2 - \frac{1}{2}k_y^2 : -u_{tx} = c\left(u_{xx} + \frac{1}{2}u_{yy}\right)$$

Note that the transmitted wave is $U_{tr} = Te^{i(ax+by)}$ where $k^2 = a^2 + b^2$ where a is the x-wave number of the transmitted wave, i.e.

for first order, $a = k$, $R = O(\theta^2)$ (see above), and

for second order $a = (k - 1/2k_y^2/k) = k(1-1/2\sin^2\theta)$, $R = O(\theta^4)$

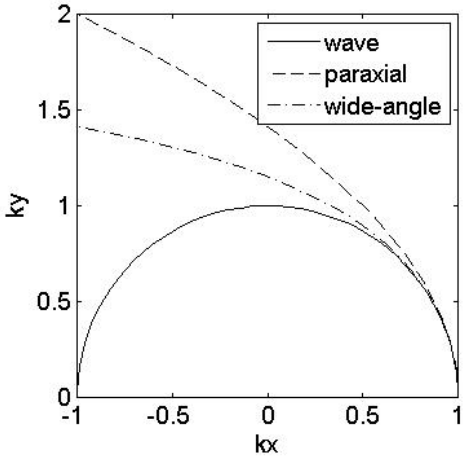
The second order condition is easily implemented on the staggered Yee grid (see copy from Taflove-Hagness)

The dispersion relation may also be used to derive the "paraxial" approximation, which allows a marching type numerical solution at the price of neglecting the back-scatter. It is useful for waveguides ("Beam propagation method"), sound transmission in stratified media, etc.

$$k_x = -k(1-\frac{k_y^2}{2k^2}) = -k + \frac{1}{2k}k_y^2 : -iu_x = -ku - \frac{1}{2k}u_{yy}$$

With $u = e^{-ikx}v, iv_x = \frac{1}{2k}v_{yy}$, the Schroedinger equation

The approximations can be illustrated in the (k_x,k_y)-plane: The circle is the wave equation dispersion relation, and the parabola is the paraxial approximation.



The "wide-angle" paraxial approximation comes from a Padé-approximation to the square root:

$$\sqrt{1-x} = \frac{4-3x}{4-x} + O(x^3),$$

giving the PDE

$$k_x = \frac{4-3k_y^2/k^2}{4-k_y^2/k^2}$$

$$-i(k^2u_x + \frac{1}{4}u_{yyx}) = (k^2u + \frac{3}{4}u_{yy})$$

4.2 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 $\mathrm{Re}\ \kappa_1 < 0$ 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

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

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 $s_1 = s_2 = 1$

4.2.1 Choice of σ 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 $s_1 = 1/s_3 = 1/s_2 = (1+\frac{\sigma}{\varepsilon j\omega})$, 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.

4.2.2 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.

4.2.3 Amount of damping; choice of σ.

From the construction, the wave number κ_x is complex,

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

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

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

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

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

so R can be made as small as we please by choice of σL.

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

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

5 Sources

Two kinds, point sources in the computational domain such as current pulses on wires, and waves (cylindrical, plane,…) created by external sources.

5.1 Point sources

A point source may be implemented as a prescribed variation of say the E-field in a point. This correctly describes the wave moving away from the source, but also creates reflections from scattered waves hitting the source. In a 1D-case, such a source is a total reflector. In cases where the scattered waves arrive later than the duration of the pulse, one can simply exchange the source for the standard update after the pulse time.

In 2 and 3D, the reflections in the source are much weaker – only in a single gridpoint and we neglect them.

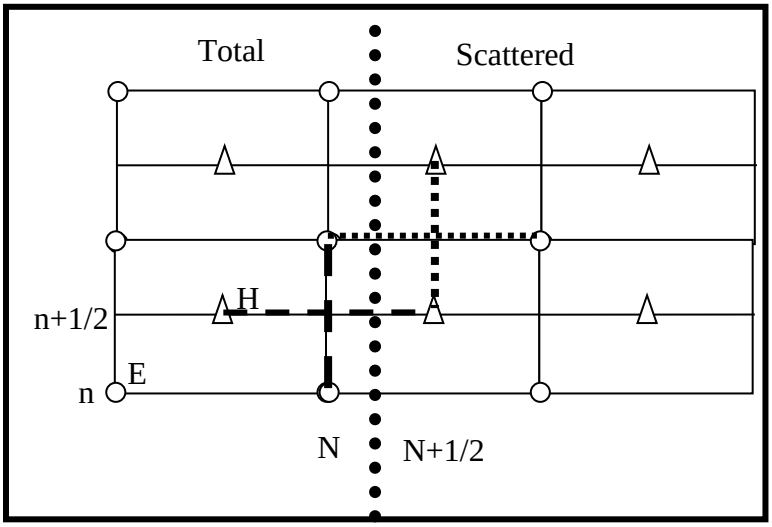
5.2 External wave sources

An externally generated wave can be implemented as initial condition, but this is a problem with persistent sources such as a harmonic wave turned on at t = 0. One usually employs "***Huygen's surfaces***" which decompose the domain into a portion outside the scatterer where only the scattered waves U_{sc} are represented on the grid, and a near-field domain where the total field, $U_{tot} = U_{inc} + U_{sc}$ sum of incoming and scattered waves is represented. We illustrate the technique on a 1D-case $\begin{matrix}\varepsilon E_t = H_x \\ \mu H_t = E_x\end{matrix}$ with an incoming wave $\mathbf{U}_{\mathrm{inc}}(x,t) = \begin{pmatrix} E_{inc}(x,t) \\ H_{inc}(x,t)\end{pmatrix}$ and the Yee-scheme. Let the exterior domain be $x > x_{N+1/4}$ (note: the surface is between x_N and $x_{N+1/2}$) so that variables with subscripts >= N+1/2 mean scattered field and with subscripts <= N mean total field.

$$\varepsilon\frac{E_k^{n+1}-E_k^n}{\Delta t} = \frac{H_{k+1/2}^{n+1/2}-H_{k-1/2}^{n+1/2}}{\Delta x}$$

$$\mu\frac{H_{k+1/2}^{n+1/2}-H_{k+1/2}^{n-1/2}}{\Delta t} = \frac{E_{k+1}^{n}-E_{k}^{n}}{\Delta x}$$

is used for k <= N-1/2 and k >= N+1



The update equations for E_N and $H_{N+1/2}$ become:

$$\varepsilon\frac{E_N^{n+1}-E_N^n}{\Delta t}=\frac{H_{N+1/2}^{n+1/2}-H_{N-1/2}^{n+1/2}}{\Delta x}+\frac{1}{\Delta x}H_{inc}(x_{N+1/2},t^{n+1/2})$$

$$\mu\frac{H_{N+1/2}^{n+3/2}-H_{N+1/2}^{n+1/2}}{\Delta t}=\frac{E_{N+1}^{n+1}-E_N^{n+1}}{\Delta x}-\frac{1}{\Delta x}E_{inc}(x_N,t^{n+1})$$

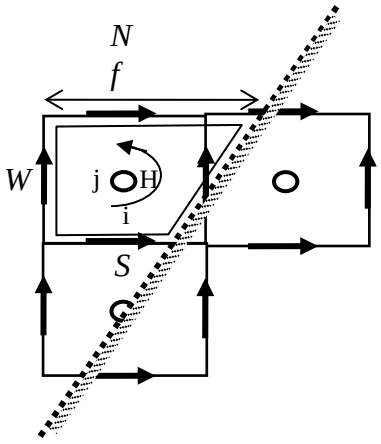
Modeling: Absorbing boundary conditions; dispersive material; fixes for staircasing
Book Ch. 5.3 pp 79- 81

6 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.

6.1 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)



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

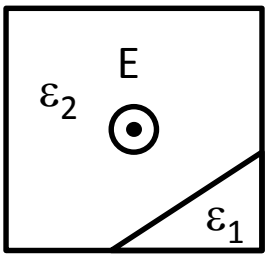
$$\mu A\frac{dH}{dt} = \Delta y E_y^W + fE_x^N - g\cdot E_x^S$$

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.

6.2 Non-aligned Dielectric boundaries

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

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



7 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!*

7.1 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*:

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

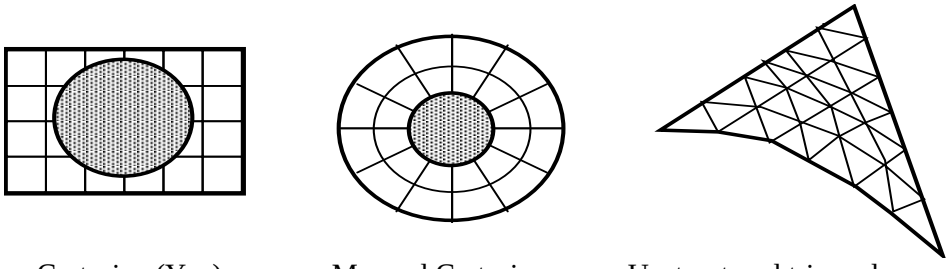
$$E^{n+1}=e^{-\frac{\sigma\Delta t}{\varepsilon}}E^n+e^{-\frac{\sigma}{2\varepsilon}\Delta t}\frac{\Delta t}{\varepsilon}\nabla\times H^{n+1/2}$$

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,

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

8 Geometry and grid methods

We have seen the Yee-scheme, and how to treat sources and boundary conditions. In all, the Yee scheme is extremely successful. Its drawback is the necessity for a rectangular equi-sized grid: Non-rectangular geometry has to be approximated by LEGO-style bricks, sometimes also referred to as staircase effect.
Finite Volume and Finite Element methods for dealing with curvilinear geometry have been used for e.g. computational fluid dynamics since the sixties. Common grid types are shown here:



Cartesian (Yee) Mapped Cartesian Unstructured triangular

It is natural to investigate how such schemes can be used for the Maxwell equations as well: Existing pre- and post-processing software, and some of the solvers developed for CFD, could be re-used. This lecture gives an overview of how the various issues have been addressed.

Difficulties in standard approaches applied to the Maxwell equations

• There are waves running both right and left and symmetric schemes are natural. However standard central difference schemes are prone to odd/even decoupling, i.e., oscillatory numerical solutions that oscillate with the shortest wavelength representable on the grid. These waves are sometimes referred to as "spurious modes" and can also be associated with the dispersion, wavelength $2\Delta x$ perturbations travel at speed 0.
In steady CFD the remedy is to add a controlled amount of numerical dissipation, by artificial viscosity or diffusion, or even fourth order difference terms.

• An alternative is the use of (unsymmetric) upstream differences. This requires essentially that the system be diagonalized, which is easy when the coefficients are piecewise constant. But first order schemes are much too dissipative, and better than first order accuracy requires complicated schemes. Note that it is much easier to devise good schemes for the second order wave equation formulation because of the compactness of the second difference formula. But often both $\boldsymbol{H}$ and $\boldsymbol{E}$ are necessary, e.g. for modeling dispersive and non-linear media, and in such cases the wave equation formulation thus is slightly more cumbersome.

For spatially multidimensional cases there is also another source of spurious solutions:
• Artificial growth of non-solenoidal components of $\boldsymbol{B}$ and $\boldsymbol{D}$, i.e., violation of (proper discrete variants of) the Gauss laws. This does not happen in the Yee scheme but may in second order wave equation formulations, or in approximations to curl curl unless the scheme is properly designed – see Andre's lecture Oct 9. This is related to "long time instability", which is often a linear growth of the error:

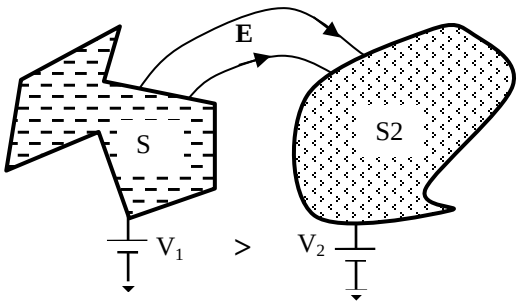
9 Integral equation methods in the frequency domain

Book p 154 – 198

9.1 Introduction - electrostatics

Let us start by discussing a "Newtonian" view of electromagnetics – focusing on the charges, the sources of the fields, and then compare it with the "Laplacian" PDE view. The Coulomb force between two charges Q_i and Q_j at $\mathbf{x}_1$ and $\mathbf{x}_2$ is

$$\mathbf{F}_{ij} = \frac{1}{4\pi\varepsilon}\cdot\frac{Q_i Q_j}{R_{ij}^3}(\mathbf{x}_i - \mathbf{x}_j), R_{ij} = \left|\mathbf{x}_i - \mathbf{x}_j\right|$$



4π is the solid angle and ε is the dielectric constant of the medium. With n charges, the force on Q_i is

$$\mathbf{F}_i = \frac{Q_i}{4\pi\varepsilon}\cdot\sum_{j\neq i}\frac{Q_j}{R_{ij}^3}(\mathbf{x}_i - \mathbf{x}_j) = Q_i\cdot\underbrace{-\nabla V(\mathbf{x}_i)}_{\mathbf{E}(\mathbf{x}_i)},$$

$$V(\mathbf{x}) = \frac{1}{4\pi\varepsilon}\sum_{j\neq i}\frac{Q_j}{\left|\mathbf{x}-\mathbf{x}_j\right|}$$

The "electrostatic problem" calls for determination of the electric field created by a number of conductors S_i, with given potentials V_i . Only the surfaces carry charges, which will rearrange themselves on the surfaces, driven by the forces. One might try solving the many-body initial value problem

$$m_i \cdot \frac{d^2\mathbf{x}_i}{dt^2} + D\frac{d\mathbf{x}_i}{dt} = Q_i\mathbf{E}_t, i = 1,2,...,n$$

where $\mathbf{E}_t$ is the tangential component of the **E**-field acting on point *i*, computed from the positions of all the charges. The damping *D* is necessary; without it, the system would oscillate for ever. Equilibrium obtains when the net force (proportional to **E**) is orthogonal to the conducting surface. Since **E** is the gradient of *V*, the tangential component of the gradient of *V* vanishes so *V* becomes constant on the surface.
The total charge on each body is determined by the initial data. The potential is computable by integration along the **E**-field lines from "infinity", but there is no easy way to determine what the charge on each body should be to produce a desired potential.

In the Laplacian description, one solves the partial differential equation satisfied by *V*:

$$\Delta V(\mathbf{x}) = 0$$

except at $\mathbf{x} = \mathbf{x}_i$. Surrounding $\mathbf{x}_i$ by a sphere S_δ of radius δ, the formula for the field from a point charge gives

$$\int_{S_\delta} \varepsilon \nabla V \cdot \hat{n} dS = \frac{Q_i}{4\pi} \iint_{\theta,\phi} \frac{\partial}{\partial r}\left(\frac{1}{r}\right)_{r=\delta} \delta d\theta \cdot \delta \sin\theta d\phi = \frac{Q_i}{4\pi} \iint_{\theta,\phi} \frac{1}{\delta^2} \delta d\theta \cdot \delta \sin\theta d\phi = Q_i$$

By superposition, we can write

$$\varepsilon \Delta V(\mathbf{x}) = \sum_{j=1}^{n} Q_j \cdot \delta(\mathbf{x} - \mathbf{x}_j)$$

where δ is the Dirac delta-function. For a continuous charge distribution $\rho(\mathbf{x})$ this becomes

$$\varepsilon \Delta V(\mathbf{x}) = \int \rho(\mathbf{x}')\delta(\mathbf{x} - \mathbf{x}')dV = \rho(\mathbf{x})$$

whereas the "Newtonian" description is

$$V(\mathbf{x}) = \int \frac{\rho(\mathbf{x}')}{4\pi\varepsilon|\mathbf{x} - \mathbf{x}'|} dV'$$

The solution *G* of

$$\Delta_{\mathbf{x}} G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}'), G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi|\mathbf{x} - \mathbf{x}'|}$$

(the subscript on the differential operator shows differentiation w.r.t **x**, not **x**') is called the Green's function for the free space Laplace operator with boundary condition $G = 0$ at infinity. Note that:

- the differential equation has constant coefficients, so *G* depends only on the difference $\mathbf{x} - \mathbf{x}'$;
- the isotropy of the differential operator (actually, rotational invariance) makes *G* a function only of the distance $|\mathbf{x} - \mathbf{x}'|$

For the electrostatic problem with given conductor potentials, the charge is a surface charge σ and we have

$$V(\mathbf{x}) = \int_S \sigma(x')G(\mathbf{x}, \mathbf{x}')dS, \quad S = \bigcup S_i$$

$$V_k = \int_S \sigma(\mathbf{x}')G(\mathbf{x}, \mathbf{x}')dS, \mathbf{x} \in S_k, k = 1,2,..., n_{cond.}$$

a "first kind Fredholm" integral equation for the unknown σ. We know from potential theory that the Laplace/Poisson problem has a unique solution. Since we can calculate σ from the normal component of the **E**-field,

$$\sigma = \varepsilon \frac{\partial V}{\partial n}$$

we expect the integral equation to have a unique solution too. But First Kind equations are known for their ill-conditioning. Consider solving

$$f(x) = \int_I u(y)K(x,y)dy$$

for *u*. If the kernel function *K* is smooth, the integral operator smooths short wavelength variations in *u*. The converse is that rapid variation in *f*, such as e.g. measurement noise, is magnified in *u*. If the magnification is NOT uniformly bounded, such a problem is called ill-posed and requires filtering, *regularization*. However, the point charge kernel function has an integrable 1/*r*-type singularity for **x** close to **x**'– not so smoothing, yet nice enough. In 2D, the Green's function is $-\frac{1}{2\pi}\ln(\mathbf{x}-\mathbf{x}')$ and the story is similar.

Notes
The $O(h)$ error observed is not obvious: The exact solution has an $r^{-1/2}$ type singularity at external right angled corners. Thus, the numerical solution cannot converge uniformly pointwise (but it can in l_2 – norm). When convergence is regular, one can improve the results by Richardson extrapolation:

$$\left.\begin{aligned} C(h) &= C + Kh + O(h^2) \\ C(2h) &= C + 2Kh + O(h^2) \end{aligned}\right\} \Rightarrow C = C(h) + (C(h) - C(2h)) + O(h^2)$$

Capacitor example from Book: The extrapolated value from 10 and 20 elements is 18.71 which has only 0.1% error and is much better than the result with 200 elements.

9.2 Scattering of TM$_z$ waves from perfectly conducting objects.

The development above indicates that any electrostatic field between conductors can be produced by some charge distribution on their surfaces. So maybe *any* solution to the Laplace equation in a closed domain *D* with *exterior* normal ***n*** can, too? The answer is yes, but one needs both a single-layer charge σ and a layer of *dipoles*, say γ. The argument runs as follows: Consider a modified domain *D*', equal to *D* excluding a small sphere S_δ around a point **x** and a tube connecting S_δ to the boundary of *D*. The surface of *D*' is *S*'. Let *u* be a solution to the Laplace equation in *D*, and $v(\mathbf{x}') = G(\mathbf{x},\mathbf{x}')$.
Then

$$0 = \int_{D'} (u\Delta v - v\Delta u)dV = \int_{S'} \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n} \right) dS =$$

$$\int_{S'-S_\delta} \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n} \right) dS + \underbrace{\int_{S_\delta} u\frac{1}{4\pi\delta^2}\delta^2 \sin\theta d\theta d\phi}_{\to u(x)} - \underbrace{\int_{S_\delta} \frac{1}{4\pi\delta}\cdot\frac{\partial u}{\partial n}\delta^2 \sin\theta d\theta d\phi}_{\to 0}$$

as δ -> 0. Finally, we obtain the representation

$$u(\mathbf{x}) = \int_S \left(u(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'} - G(\mathbf{x},\mathbf{x}')\frac{\partial u}{\partial n}(\mathbf{x}') \right) dS$$

The same representation is valid for solutions to the Helmholtz equation, for which the Green's function in 3D is

$$G(\mathbf{x}.\mathbf{x}') = \frac{1}{4\pi}\frac{e^{-ikR}}{R},\ R = |\mathbf{x}-\mathbf{x}'|$$

(see notes for the 2D formula).

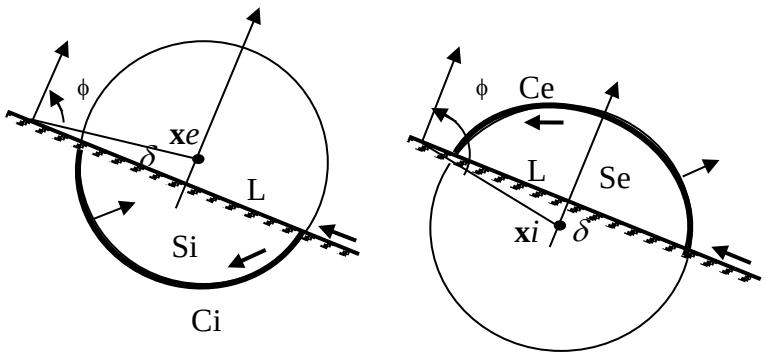
The formula

$$u(\mathbf{x}) = \int_S \left(\sigma(\mathbf{x}')G(\mathbf{x},\mathbf{x}') - \gamma(\mathbf{x}')\frac{\partial G(\mathbf{x},\mathbf{x}')}{\partial n'} \right) dS \qquad (*)$$

defines a solution to the Helmholtz equation both inside and outside *S*. Let the exterior to *S* be *e* and the interior *i*. Due to the singularity of *G* and its derivatives, *u* and its normal derivative jump across *S*:

$$u(e) - u(i) = \gamma, \partial u/\partial n(e) - \partial u/\partial n(i) = \sigma \qquad (**)$$

Here is a proof of the first jump relation, for ease of illustration, for the Laplace operator in 2D. Assume that *u* is continuously differentiable everywhere. Potential theory guarantees that it will be more than that, actually analytic, except possibly on the boundary at corners, etc.



The exterior viz. interior points **x**e and **x**i, at distance δ from *S*, are surrounded by circular disks of radius *a*.

As δ vanishes, $\int_S \sigma(x')G(xe,x')dS$ and $\int_S \sigma(x')G(xi,x')dS$ converge to the same limit so σ does not contribute to the jump in *u* (but for *du*/*dn* it does). For the γ-term, we need the expression for *dG*/*dn*:

$$v = \partial G/\partial n' = \nabla G \cdot \mathbf{n}' = dG/dR\left(\nabla R \cdot \mathbf{n}'\right) = \frac{1}{2\pi R}\cos\phi$$

For **x**e,

$$u(xe) = \int_S v_e(x')u(x')ds = \int_{S-L} v_e(x')u(x')dS + \int_L v_e(x')(u(x') - u(x^*))dS + u(x^*)\int_L v_e(x')ds =$$

$$= \int_{S-L} v_e(x')u(x')dS + \underbrace{\int_L v_e(x')(u(x') - u(x^*))dS}_{Q_e, |Q_e| \le Ka} + u(x^*)\underbrace{\int_{Ci} v_e(x')ds}_{-\alpha_e(a,\delta)/2\pi}$$

where α_e is the subtended angle from **x**e to the intersection of the circle with *S*. The Gauss theorem was used:

$$0 = \int_{Si} \Delta G dS = -\int_{Ci} \partial G/\partial n' dS + \int_L \partial G/\partial n' dS;\ \int_{Ci} v(x')dS = \int_L v(x')dS$$

For **x**i

$$u(xi) = \int_S v_i(x')u(x')dS = \int_{S-L} v_i(x')u(x')dS + \underbrace{\int_L v_i(x')(u(x') - u(x^*))dS}_{Q_i, |Q_i| \le Ka} + u(x^*)\underbrace{\int_{Ce} v_i(x')ds}_{+\alpha_i(a,\delta)/2\pi}$$

Note the different sign on α! There follows

$$u(xe) - u(xi) = \int_S (v_e(x') - v_i(x'))u(x')dS + Q_e - Q_i + (-\alpha_e - \alpha_i), |Q| \le Ka$$

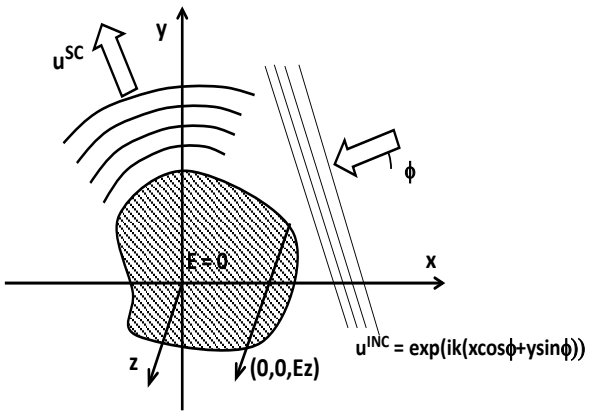
and as δ and *a* vanish, v_e and v_i approach a common limit so the integral vanishes because *u* is bounded, and the sum of α_e and α_i approach 2π, which ends the demonstration. (as usual, modulo the sign +/-)

10 Scattering of plane wave on metallic circular cylinder

We consider time-harmonic TM-waves of angular frequency ω in the plane. The only non-zero E-component is E_z which we call *u*, and it satisfies the Helmholtz equation

$\Delta u + k^2 u = 0, k = \frac{2\pi}{\lambda} = \frac{\omega}{c} = \omega\sqrt{\varepsilon\mu}$ in the exterior domain. On Γ, the tangential E-field is zero, i.e., the sum of the incoming field and the scattered field vanishes,

$$u^{INC} + u^{SC} = 0$$



Any solution of the Helmholtz equation can be represented by an integral over *Γ*,

$$u^{SC}(x) = \int_\Gamma \left(G(x,x')\sigma(x') - \frac{\partial G(x,x')}{\partial n'}\gamma(x') \right) ds$$

where *G* is the Green's function, satisfying

$$\Delta_x G(y,x) + k^2 G(y,x) = \delta(x-y)$$

with δ the Dirac delta-function. σ and γ are single layer and double layer sources, viz., on Γ. For the exterior wave problem, *G* must be an outgoing wave at infinity, and thus must be the zeroth order Hankel function of the second kind,

$$G(y,x) = \frac{1}{4i} H_0^2\left(k\,|\,y-x\,|\right)$$

Note that *G* is a function only of the difference $y - x$ and that it has a logarithmic singularity at $x - y = 0$.

Consider now the integral evaluated for points e and i just outside and just inside Γ. The jumps in function value [u^{SC}] and normal derivative [$\partial u^{SC}/\partial n$] are

$$u^{SC}(e) - u^{SC}(i) = \gamma,\ \partial u^{SC}/\partial n(e) - \partial u^{SC}/\partial n(i) = \sigma$$

Define the scattered field to be continuous across Γ. This is possible whenever the interior Helmholtz problem with Dirichlet condition has a unique solution. This, in turn, holds whenever $-k^2$ is NOT an eigenvalue of the Laplace operator inside Γ, i.e., for all but a number of discrete values of k^2. Then $\gamma = 0$ and the final integral equation for determining σ becomes

$$u^{INC}(x) = \int_\Gamma \sigma(x')G(x,x')ds$$

This is a "Fredholm integral equation of the first kind" with kernel *G*. First kind equations with smooth kernels are often ill-posed in the sense that short wavelength perturbations to σ are smoothed by the integration. The converse of this statement is that short wavelength components of the LHS are strongly magnified. Such problems have to be regularized by filtering out short wavelength noise.

However, our kernel *G* is (weakly) singular and $\sigma(x)$ contributes strongly to $u^{INC}(x)$. The problem of determining σ from u^{INC} is reasonably well conditioned.

There remains to discretize the integral equation to produce a finite linear system of equations. We will use the collocation method which proceeds by approximating σ by a linear combination of a number of selected basis functions,

$$\sigma(y) \approx \sum_{k=1}^{n} \sigma_k f_k(y)$$

selecting a number of field points z_k just outside Γ and requiring that the equation be satisfied exactly at these points:

$$b_m := u^{INC}(z_m) = \sum_{k=1}^{n} \sigma_k \int_{\Gamma} f_k(z') G(z_m, z') ds, z_m \in \Gamma(e), m = 1,2,...,M$$

or

$$\mathbf{As} = \mathbf{b}\,,\ a_{km} = \int_{\Gamma} f_k(z') G(z_m, z') ds$$

where M is usually chosen = n but may also be taken > n to provide some over-determination in ill-conditioned cases.

The simplest basis functions are constructed by replacing the curve Γ by a polygon with vertices z'_k, edges $\Delta z_k = z'_{k+1} - z'_k$. We take $f_k = 1$ over edge k, 0 elsewhere, the "square pulse" basis functions which give a staircase representation of $\sigma(x)$. z_k are usually chosen as the midpoints of the edges,

$$z_k = 1/2(z'_{k+1} - z'_k)$$

The integrals are evaluated exactly, if possible, or by numerical quadrature. The simplest scheme is to use a one-point rule for all integrals except for $k = m$, the self-contribution of element m, which becomes the diagonal element of the coefficient matrix A.

This is a logarithmic singularity and we choose to use only the first few terms in the expansion of G around z_m: (from e.g. Maple or Mathematics Handbook)

$$H_0^2(z) = J_0(z) - iY_0(z) \approx 1 - i\left(\frac{2}{\pi}\{\ln\left(\frac{1}{2}z\right) + \gamma\}\right) + O(z^2 \ln z), \gamma = 0.5772156649...$$

$$G(z) = \frac{1}{4i} H_0^2(z) \approx \frac{1}{4i} - \frac{1}{2\pi}(\gamma - \ln 2) - \frac{1}{2\pi}\ln z$$

Note the last term: This is the Green's function for the Laplace operator.

10.1 Field computation for the Helmholtz equation in 2D

We have seen that the field may be written

$$E(z) = \int_{\Gamma}\left(G(|z - z'|)\sigma(z') - \gamma(z')\frac{\partial G(|z - z'|)}{\partial n'}\right)ds$$

where the Green's function is $G(r) = \frac{1}{4i} H_0^2(kr)$, the zeroth order Hankel function of the second kind.

Primed quantities refer to the curve, **n**' is the normal to the curve Γ and ds is the arc element. The coordinates are represented as complex numbers, $z = x + iy$, etc.

Γ is approximated by a polygon with vertices z'_i, i = 1,…, M, and the field points are z_i, i = 1,…, n. Using the fact that G is a function of k times the length |z - z'| only we may write

$$\gamma\frac{\partial G}{\partial n'}ds = \nabla' G\cdot\mathbf{n}'\gamma ds = -kG'(k|z-z'|)\frac{z-z'}{|z-z'|}\cdot\gamma\frac{i\Delta z'}{|\Delta z'|}ds =$$

$$= kG'(k|z-z'|)\gamma\frac{\mathrm{Re}((z-z')i\bar{\Delta}z')}{|z-z'|}$$

where the normal is i times tangent and the scalar product can be expressed

<z1,z2> = Re(z1 conj(z2))

Let the midpoints of the polygon edges be $z'_{i+1/2}$ and $d_i = z - z'_{i+1/2}$., $\Delta_j = z'_{i+1} - z'_i$. The final formula becomes

$$E(z) = \sum_{j=1}^{n}\sigma_j G(k\mid d_j\mid)|\Delta_j| + \gamma_j kG'(k\mid d_j\mid)\frac{\mathrm{Re}(id_j\bar{\Delta}_j)}{\mid d_j\mid}$$

This is implemented by the m-file below, vectorized to compute the field on a mesh of *m* x *n* z-points at once.

Exercise

1. Compute σ and γ (as $\partial u/\partial n$ and u) for u^{SC} = a plane wave e^{ikx} on a closed curve of your choice. Plot the field from σ and γ inside and outside the circle. Explain.

2. The polygon edges $\Delta_j = z'_{i+1} - z'_i$ must be small enough to resolve the wavelength. Compare the fields computed in 1. with 5, 10, and 20 elements per wavelength

3. The code is completely vectorized (no loops) but needs memory `ns*m*n` which easily becomes huge. Rewrite the code to use only a given amount of memory by cutting the set of z-points into reasonable size chunks, with a single loop over the chunks. The code is also wasteful in allocating space both to `d,G`, and `Gder`. At least one can be discarded without speed penalty. Fix that too.

```
function E = field(z,zprime,gamma,sigma,k)
% computes the field at the points z(1:np) (2D: z(p) = x(p) + i y(p))
% from the
% single layer  sigma(1:ns-1) and
% double layer  gamma(1:ns-1)
% on the curve  zprime(1:ns).
% Greens function for the Helmholtz (Laplace if k = 0) equation
% (delsq + k^2)u = ...
% and all of R2 i.e. H2,0(k|z - zprime|) viz. 1/(2pi) ln (|z-zprime|)
%r
[m,n]  = size(z);
ns     = length(zprime);
np     = m*n;
z      = z(:);                                    % make columns
gamma  = gamma(:);
sigma  = sigma(:);
zprime = zprime(:);

delta  = diff(zprime);                            % edges
zphalf = 0.5*(zprime(1:ns-1) + zprime(2:ns));     % midpoints
d      = z*ones(1,ns-1) - ones(np,1)*(zphalf.'); % all distance vectors
                                                  % at once
G      = greenfunc(k,d);                          % single layer Green
Gn     = k*greenfuncder(k,d);                     % double layer Green
sig    = sigma.*abs(delta);                       % length element
```

```
E      = reshape(G*sig -
(Gn.*real(1i*d./abs(d)*diag(conj(delta))))*gamma,m,n);

function G = greenfunc(k,r)
if k == 0 % Laplace
      G = 1/2/pi * log(abs(r));
else
      G = -0.25*i*besselh(0,2,k*abs(r));
end

function G = greenfuncder(k,r)
if k == 0 % Laplace
      G = (1/2/pi)./abs(r);
else
      G = 0.25*i*besselh(1,2,k*abs(r));
end
```

10.2 Exact solutions

The code in the lab will work for any curve defined by the *z'*-points. For a circle of radius *R* we can compute the exact solution by Fourier expansion.

PEC cylinder radius R

The exterior field is

$$u^{SC}(r,\phi) = \sum_{m=-\infty}^{+\infty} c_m e^{im\phi} H_m^2(kr)$$

and the incoming plane wave may be written

$$u^{INC}(R,\phi) = e^{ikR\cos\phi} = \sum_{m=-\infty}^{+\infty} i^m J_m(kR) e^{im\phi}$$

so we obtain from $u^{\mathrm{SC}} + u^{\mathrm{INC}} = 0$ on $r = R$

$$u^{SC}(r,\phi) = \sum_{m=-\infty}^{+\infty} \underbrace{(-i^m J_m(kR)/H_m^2(kR))}_{c_m} e^{im\phi} H_m^2(kr)$$