Lecture 1
Mathematics of the Maxwell equations
References: Taflove, Jackson, …

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

J.C.Maxwell, 1867: $$\frac{\partial \mathbf{D}}{\partial t} - \nabla \times \mathbf{H} + \mathbf{J}_e = 0; \nabla \cdot \mathbf{D} = \rho$$

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

	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	J_e A/m^2	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 div **D** = div **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 by Prof. He's lectures.

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),* ***Lab 1*** FVTD e.g. Shang FETD Bondesson	FEFD (many)
Integral	Chew, Illinois (1998?)	*MoM (Harrington 1968)* *Rao, Glisson, Wilson,* ***Lab 2*** Nedelec, Monk, …
Rays	-??	Keller – only overview

Interface conditions
see homework.

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

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

$$\gamma_i = \frac{S_{x_i}}{\sqrt{\sum \left(S_{x_i}\right)^2}} = \cos\phi_i$$

$$\text{Non} - \text{trivial solutions}: \mathbf{a} \text{ must be an eigenvector and } -\lambda \text{ the corresponding eigenvalue.}$$

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

$$\text{for any real } \{\gamma_i\}.$$

Normal to surface is $(\gamma_1, \gamma_2, .., \gamma_n, \lambda)$. The front moves in its normal direction with phase-speed –λ. For

$$dS = S_t dt + \sum dx_i S_{x_i} = 0. \text{ Take } dx_i = \gamma_i \delta \text{ (small displacement in normal direction).}$$

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

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 orthogonal 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
Waves moving in the (*x*,*y*)-plane, H-field **H** = (0,0,*H*),

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

$$\mathbf{u} = \begin{pmatrix} E_x \\ E_y \\ H \end{pmatrix} : \mathbf{u}_t + \mathbf{A}_1 \mathbf{u}_x + \mathbf{A}_2 \mathbf{u}_y = 0, \mathbf{A}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1/\varepsilon \\ 0 & 1/\mu & 0 \end{pmatrix}, \mathbf{A}_2 = \begin{pmatrix} 0 & 0 & -1/\varepsilon \\ 0 & 0 & 0 \\ -1/\mu & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} \lambda & 0 & -\gamma_2/\varepsilon \\ 0 & \lambda & \gamma_1/\varepsilon \\ -\gamma_2/\mu & \gamma_1/\mu & \lambda \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0; \lambda^2{}_{1,2} = \frac{\gamma_1^2 + \gamma_2^2}{\varepsilon\mu} = \frac{1}{\varepsilon\mu}, \lambda_3 = 0$$

Speed of light $c = \frac{1}{\sqrt{\varepsilon\mu}}$, independent of direction, isotropic
Three different kinds of "waves"
$\mathbf{a}_3 = (\gamma_1, \gamma_2, 0)^T$, E - field parallel to wavefront normal, no magnetic field, electrostatic.
$\mathbf{a}_{1,2} = (\gamma_2, -\gamma_1, \pm\mu)^T$, E - field, H normal to wavefront normal. Two waves moving at *c*

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.

Lecture 2
Basics of Difference Schemes for Wave Problems
References: H-O.Kreiss, B.Gustafsson, J.Oliger: Time-Dependent Problems

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

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

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

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

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 studied in Taflove (handout) 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

$$u_t + a u_x = 0$$

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.

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

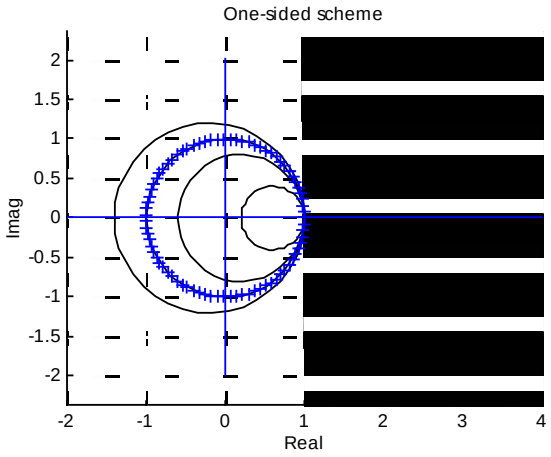
$$G = 1 + \sigma(\theta^2/2 - i(\theta - \theta^3/6)) + O(\theta^4)$$

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

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

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

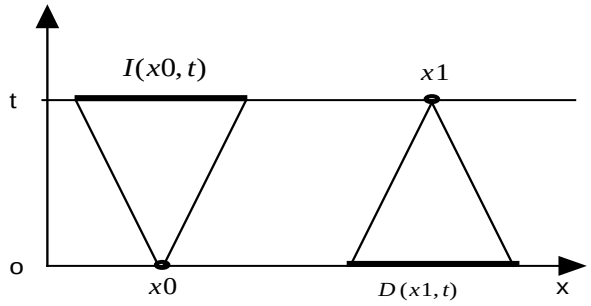
which is damped for $0 < \sigma < 1$ and unstable for other σ. It appears that the difference scheme should be chosen to reflect the direction of the characteristics: *upwind* or *upstream* differencing is useful. Why this is so can be illustrated by the

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

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

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.



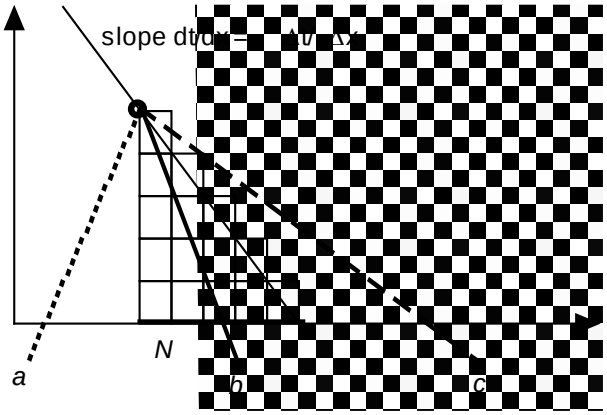
Domain of dependence *D* and Influence *I* for second-order wave equation $\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0$

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 $\boldsymbol{f}(x)$ 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 below:
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.