Finite Difference Time Domain (FDTD) methods for solution of Maxwell's equations

Case Study in Simulation Sciences

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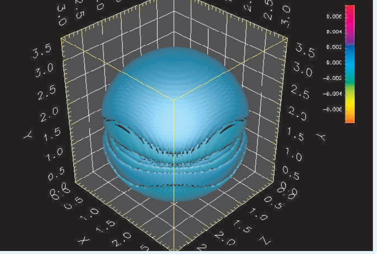

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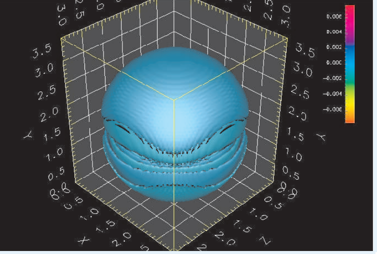

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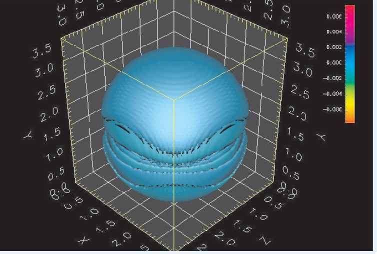

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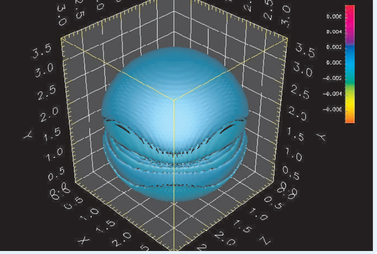

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$$\nabla \cdot \vec{B} = 0 \quad \text{(magnetic field)}$$

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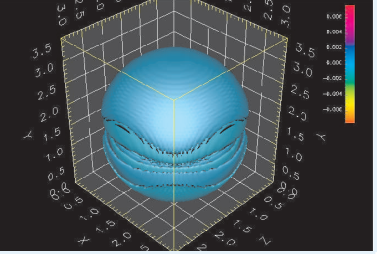

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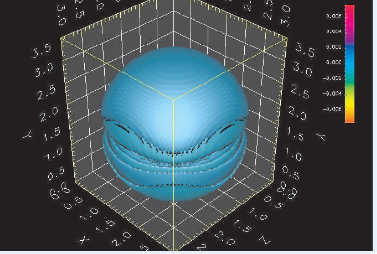
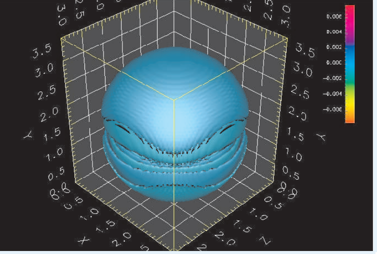
where $\vec{J} = \sigma \vec{E}$ is electric current density, ρ is total electric charge density, and the constitutive relations are given by $\vec{B} = \mu \vec{H}$ and $\vec{D} = \varepsilon \vec{E}$.



Properties of materials

μ – magnetic permeability.

$\mu = \mu_0 \cdot \mu_r$, where $\mu_0 = 4\pi \cdot 10^{-7} \frac{N}{A^2}$ is free space permeability.



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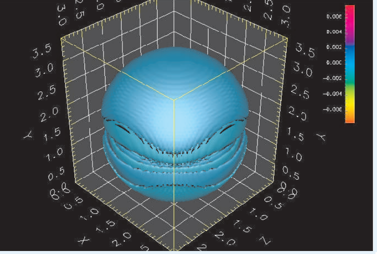

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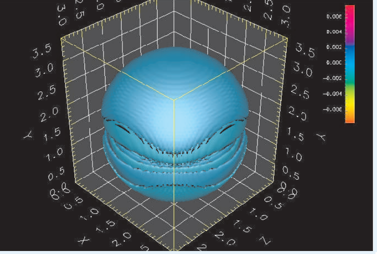
In general, μ_r and ε_r are frequency dependent. Materials without such dependence are called "the simple materials".



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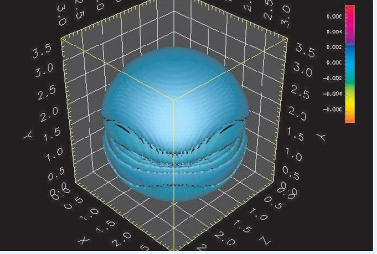

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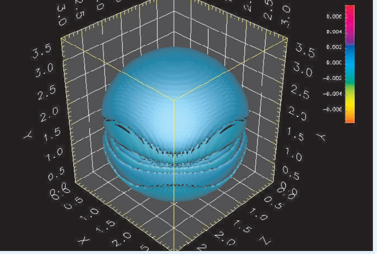

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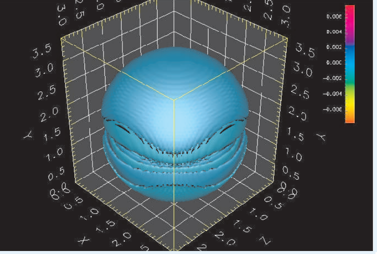
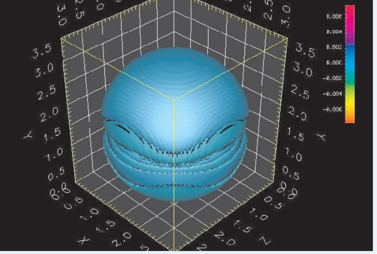
σ is electrical conductivity in $\left[\frac{S}{m}\right]$, which represents conducting properties of material.



Integral form

$$\frac{\partial}{\partial t}\iint\limits_S \vec{B}\cdot d\hat{S} = -\oint\limits_C \vec{E}\cdot d\hat{l} \quad \text{(Faraday's Law)}$$



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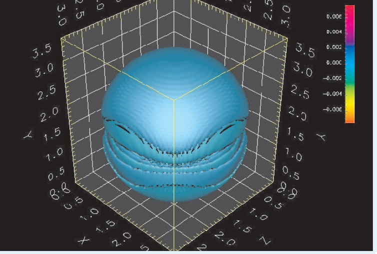

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Gauss' law:

$$\oiint\limits_S \vec{D}\cdot d\hat{S} = \iiint\limits_V \rho dV \quad \text{(electric field)}$$

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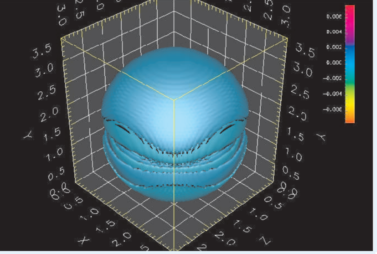


Equations in scalar form

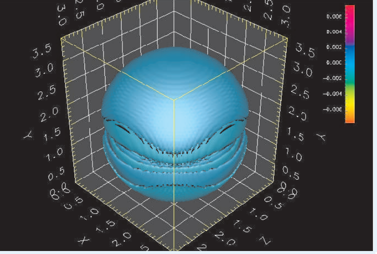
- Maxwell's Equations
- Properties of materials
- Integral form
- Equations in scalar form
- Transverse mode
- Maxwell's equations in 2D

FDTD methods

Divergence-free

Numerical stability

In Cartesian coordinates, in 3D, Maxwell's equations are



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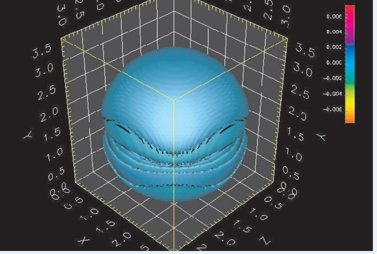

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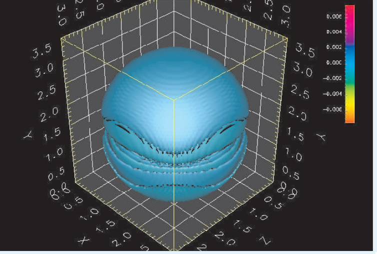
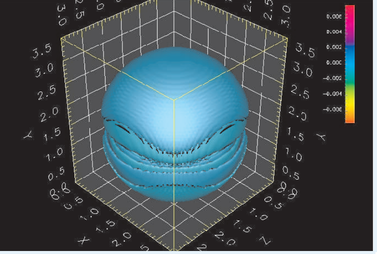
We assume that the medium is *loss-free* ($J = 0$) and ε and μ are not time-dependent)



Transverse mode

- Transverse electric (TE) modes: no electric field in the direction of propagation.



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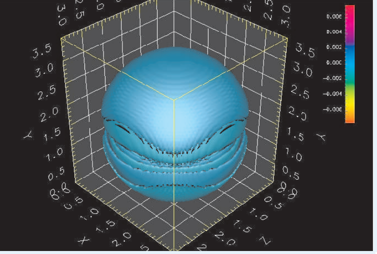

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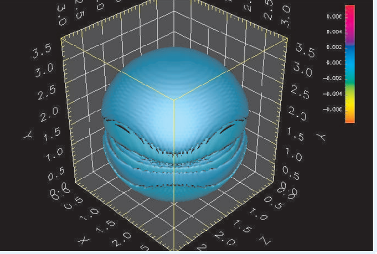

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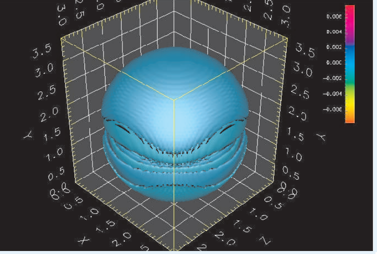

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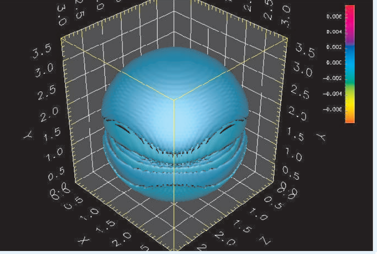

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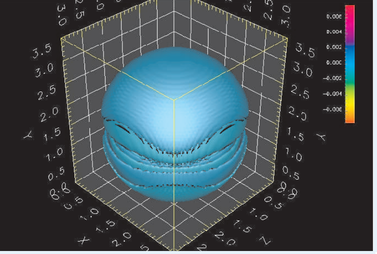
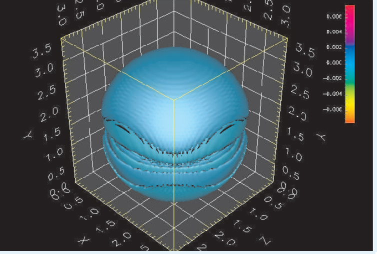
Example: a radio wave in a hollow metal waveguide must have zero tangential electric field amplitude at the walls of the waveguide, so the transverse pattern of the electric field of waves is restricted to those that fit between the walls



Maxwell’s equations in 2D

We choose z as transverse direction:



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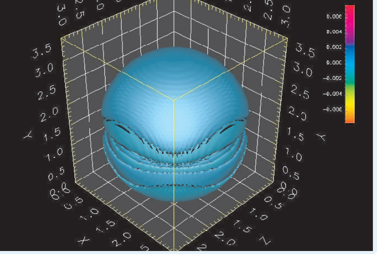

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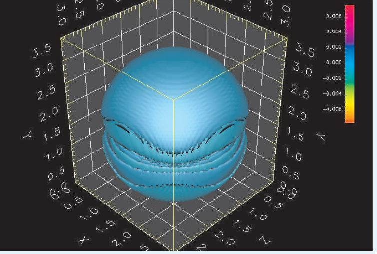
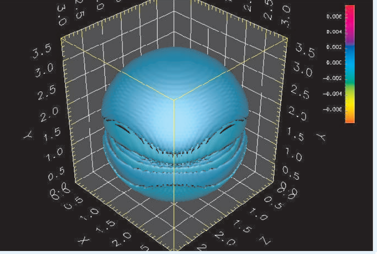


Yee Algorithm

"Classical" FDTD method (Yee, 1966) uses the second order central difference scheme for integration in space and the second order Leapfrog scheme for integration in time. This is a staggered non-dissipative scheme both in space and in time.



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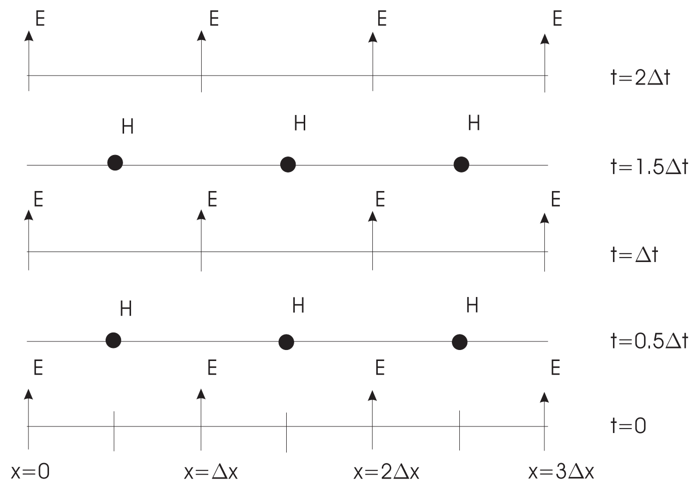
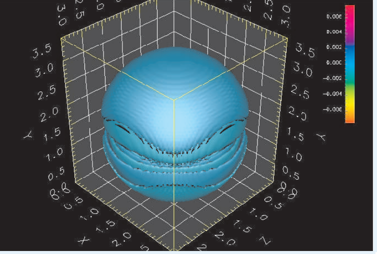


A 1D space-time chart of the Yee algorithm



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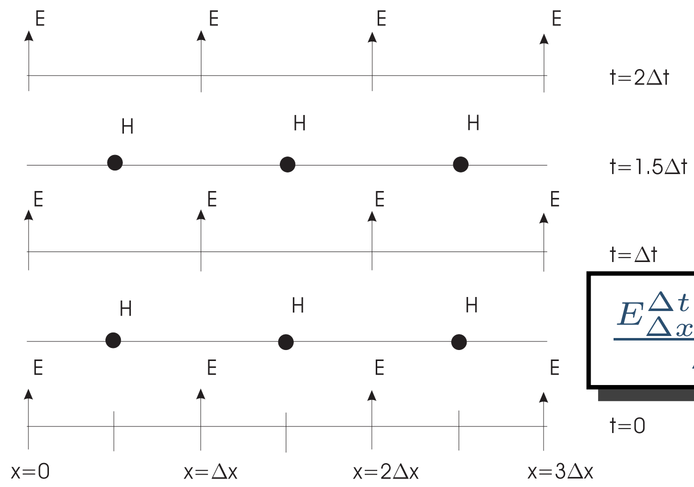

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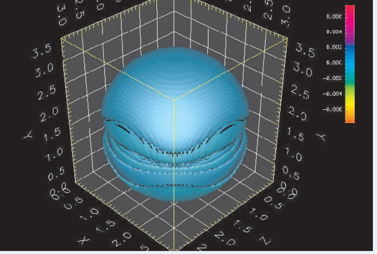

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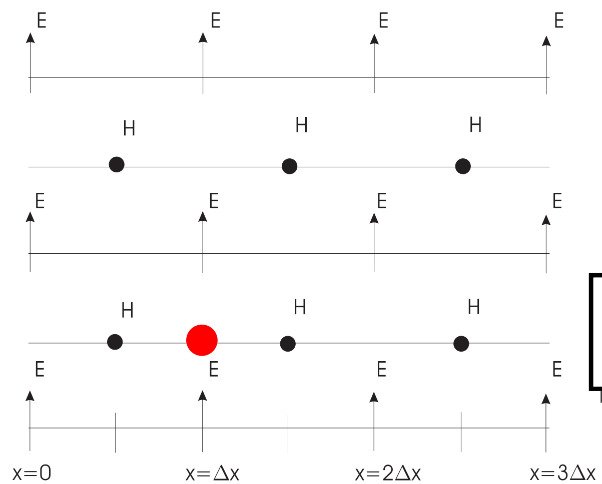

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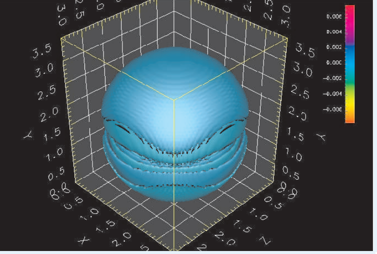
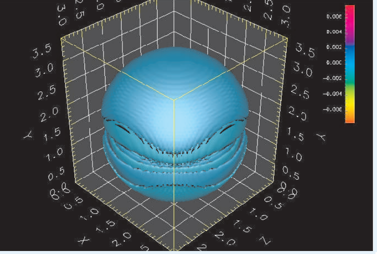


Spatial location in 3D

In Cartesian coordinates and three dimensions we have the following spatial distribution of the components:



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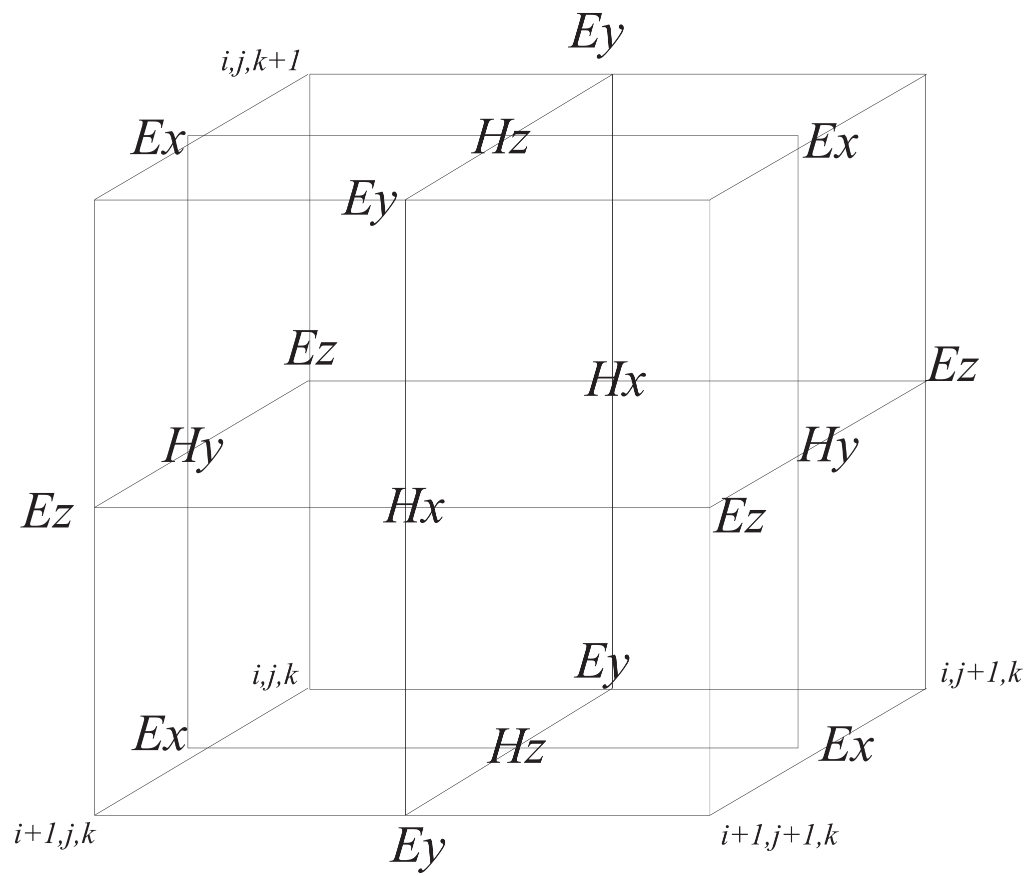
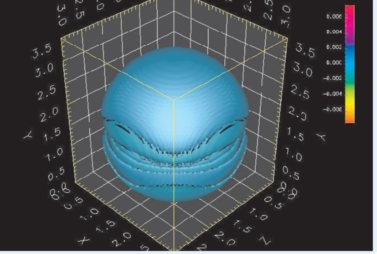




Discretization – electric field

$$E^{t+\Delta t}_{x,(i+\frac{1}{2},j,k)} = E^{t}_{x,(i+\frac{1}{2},j,k)} + \frac{\Delta t}{\varepsilon_{i+\frac{1}{2},j,k}} \Bigg[\Bigg(\frac{H^{t+\frac{\Delta t}{2}}_{z,(i+\frac{1}{2},j+\frac{1}{2},k)} - H^{t+\frac{\Delta t}{2}}_{z,(i+\frac{1}{2},j-\frac{1}{2},k)}}{\Delta y} \Bigg)$$

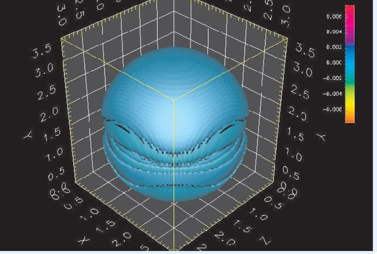
$$\Bigg(\frac{H^{t+\frac{\Delta t}{2}}_{y,(i+\frac{1}{2},j,k\frac{1}{2})} - H^{t+\frac{\Delta t}{2}}_{y,(i+\frac{1}{2},j,k-\frac{1}{2})}}{\Delta z} \Bigg)$$

$$E^{t+\Delta t}_{y,(i,j+\frac{1}{2},k)} = E^{t}_{y,(i,j+\frac{1}{2},k)} + \frac{\Delta t}{\varepsilon_{i,j+\frac{1}{2},k}} \Bigg[\Bigg(\frac{H^{t+\frac{\Delta t}{2}}_{x,(i,j+\frac{1}{2},k+\frac{1}{2})} - H^{t+\frac{\Delta t}{2}}_{x,(i,j+\frac{1}{2},k-\frac{1}{2})}}{\Delta z}$$

$$\Bigg(\frac{H^{t+\frac{\Delta t}{2}}_{z,(i+\frac{1}{2},j+\frac{1}{2},k)} - H^{t+\frac{\Delta t}{2}}_{z,(i-\frac{1}{2},j+\frac{1}{2},k)}}{\Delta x}$$

$$E^{t+\Delta t}_{z,(i,j,k+\frac{1}{2})} = E^{t}_{z,(i,j,k+\frac{1}{2})} + \frac{\Delta t}{\varepsilon_{i,j,k+\frac{1}{2}}} \Bigg[\Bigg(\frac{H^{t+\frac{\Delta t}{2}}_{y,(i+\frac{1}{2},j,k+\frac{1}{2})} - H^{t+\frac{\Delta t}{2}}_{y,(i-\frac{1}{2},j,k+\frac{1}{2})}}{\Delta x}$$

$$\Bigg(\frac{H^{t+\frac{\Delta t}{2}}_{x,(i,j+\frac{1}{2},k+\frac{1}{2})} - H^{t+\frac{\Delta t}{2}}_{x,(i,j-\frac{1}{2},k+\frac{1}{2})}}{\Delta y}$$



Discretization – magnetic field

$$H_{x,(i,j+\frac{1}{2},k+\frac{1}{2})}^{t+\frac{3\Delta t}{2}} = H_{x,(i,j+\frac{1}{2},k+\frac{1}{2})}^{t+\frac{\Delta t}{2}} + \frac{\Delta t}{\mu_{i,j+\frac{1}{2},k+\frac{1}{2}}} \times$$

$$\left[\left(\frac{E_{y,(i,j+\frac{1}{2},k+1)}^{t+\Delta t} - E_{y,(i,j+\frac{1}{2},k)}^{t+\Delta t}}{\Delta z}\right) - \left(\frac{E_{z,(i,j,k+\frac{1}{2})}^{t+\Delta t} - E_{z,(i,j+1,k+\frac{1}{2})}^{t+\Delta t}}{\Delta y}\right)\right]$$

$$H_{y,(i+\frac{1}{2},j,k+\frac{1}{2})}^{t+\frac{3\Delta t}{2}} = H_{y,(i+\frac{1}{2},j,k+\frac{1}{2})}^{t+\frac{\Delta t}{2}} + \frac{\Delta t}{\mu_{i+\frac{1}{2},j,k+\frac{1}{2}}} \times$$

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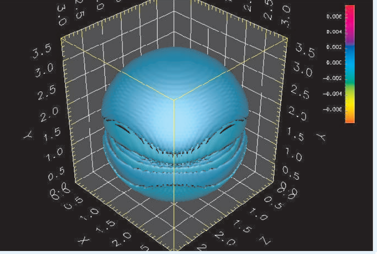
$$H_{z,(i+\frac{1}{2},j+\frac{1}{2},k)}^{t+\frac{3\Delta t}{2}} = H_{z,(i+\frac{1}{2},j+\frac{1}{2},k)}^{t+\frac{\Delta t}{2}} + \frac{\Delta t}{\mu_{i+\frac{1}{2},j+\frac{1}{2},k}} \times$$

$$\left[\left(\frac{E_{x,(i+\frac{1}{2},j+1,k)}^{t+\Delta t} - E_{x,(i+\frac{1}{2},j,k)}^{t+\Delta t}}{\Delta y}\right) - \left(\frac{E_{y,(i+1,j+\frac{1}{2},k)}^{t+\Delta t} - E_{y,(i,j+\frac{1}{2},k)}^{t+\Delta t}}{\Delta x}\right)\right]$$

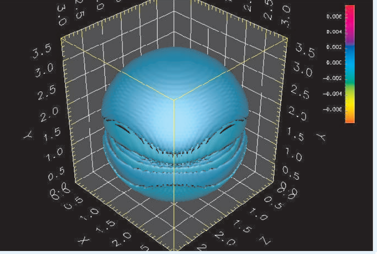


No charges, no current: $\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0$

$$\underset{\text{Yee cell}}{\oiint} \vec{D} \cdot d\hat{S} = \underbrace{\frac{\varepsilon_0}{\partial t}\left(E_{x,(i,j+\frac{1}{2},k+\frac{1}{2})} - E_{x,(i-1,j+\frac{1}{2},k+\frac{1}{2})}\right)\Delta y \Delta z +}_{\text{Term 1}}$$

$$\underbrace{\frac{\varepsilon_0}{\partial t}\left(E_{y,(i-\frac{1}{2},j+1,k+\frac{1}{2})} - E_{y,(i-\frac{1}{2},j,k+\frac{1}{2})}\right)\Delta x \Delta z +}_{\text{Term 2}}$$

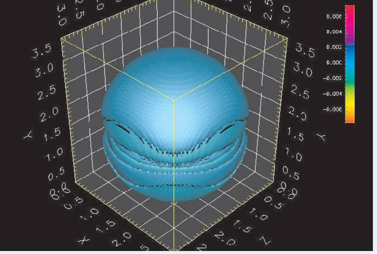
$$\underbrace{\frac{\varepsilon_0}{\partial t}\left(E_{z,(i-\frac{1}{2},j+\frac{1}{2},k+1)} - E_{z,(i-\frac{1}{2},j+\frac{1}{2},k)}\right)\Delta x \Delta y}_{\text{Term 3}}$$



Applying Yee algorithm

$$
\begin{aligned}
\mathrm{T1} = &\left(\frac{H_{z,(i,j+1,k+\frac{1}{2})} - H_{z,(i,j,k+\frac{1}{2})}}{\Delta y} - \frac{H_{y,(i,j+\frac{1}{2},j,k+1)} - H_{y,(i,j+\frac{1}{2},j,k)}}{\Delta z} \right) \\
&- \left(\frac{H_{z,(i-1,j+1,k+\frac{1}{2})} - H_{z,(i-1,j,k+\frac{1}{2})}}{\Delta y} \right. \\
&\left. - \frac{H_{y,(i-1,j+\frac{1}{2},j,k+1)} - H_{y,(i-1,j+\frac{1}{2},j,k)}}{\Delta z} \right)
\end{aligned}
$$

$$\cdots$$



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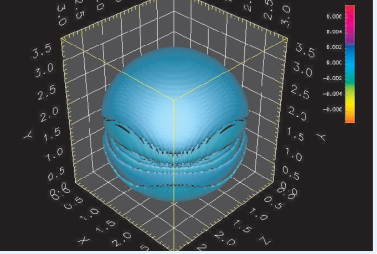
$$- \left(\frac{H_{z,(i-1,j+1,k+\frac{1}{2})} - H_{z,(i-1,j,k+\frac{1}{2})}}{\Delta y} \right.$$

$$\left. - \frac{H_{y,(i-1,j+\frac{1}{2},j,k+1)} - H_{y,(i-1,j+\frac{1}{2},j,k)}}{\Delta z} \right)$$

$$\ldots$$

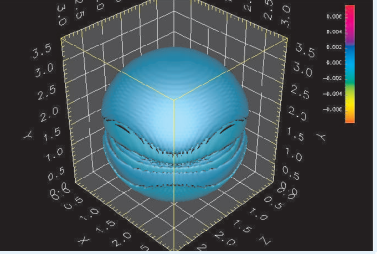
After substitution:

$$\underset{\text{Yee cell}}{\oiint} \vec{D} \cdot d\hat{S} = (\text{T1})\Delta y \Delta z + (\text{T2})\Delta x \Delta z + (\text{T3})\Delta x \Delta y = 0$$



Concept of order of accuracy

According to the **Lax-Richtmyer Equivalence Theorem**, if a finite difference scheme has a truncation error of order (p, q) and the scheme is stable, then the difference between the analytic solution and the numerical solution in appropriate norm is of order $(\Delta t)^p + h^q$ for all finite time.



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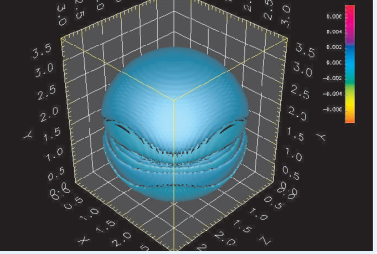
$$\frac{\partial u}{\partial x}(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = \frac{u^n_{i+1/2,j,k} - u^n_{i-1/2,j,k}}{\Delta x} + O[(\Delta x)^2] \ ,$$

$$\frac{\partial u}{\partial t}(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = \frac{u^{n+1/2}_{i,j,k} - u^{n-1/2}_{i,j,k}}{\Delta t} + O[(\Delta t)^2]$$



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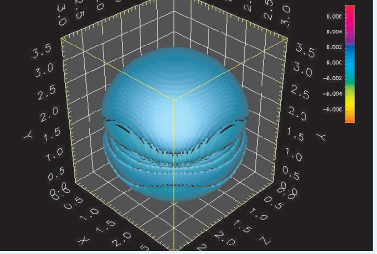
However, there is no equivalent of the Lax-Richtmyer Theorem that extends these results to approximation of equations with variable coefficients and includes boundary conditions and forcing functions*.



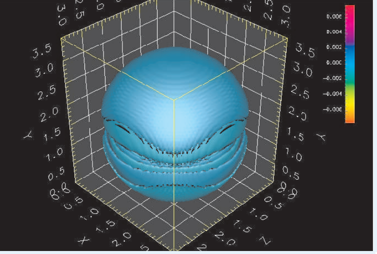
TM mode

$$\frac{H^{n+1/2}_{x,(i,j)} - H^{n-1/2}_{x,(i,j)}}{\Delta t} = -\frac{1}{\mu}\left(\frac{E^{n}_{z,(i,j+\frac{1}{2})} - E^{n}_{z,(i,j-\frac{1}{2})}}{\Delta y}\right)$$

$$\frac{H^{n+1/2}_{y,(i,j)} - H^{n-1/2}_{y,(i,j)}}{\Delta t} = \frac{1}{\mu}\left(\frac{E^{n}_{z,(i+\frac{1}{2},j)} - E^{n}_{z,(i-\frac{1}{2},j)}}{\Delta x}\right)$$

$$\frac{E^{n+1}_{z,(i,j)} - E^{n}_{z,(i,j)}}{\Delta t} =$$

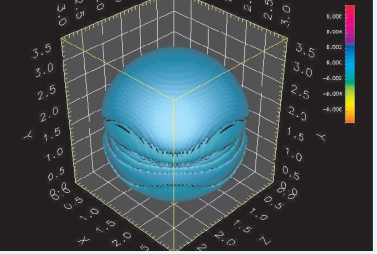
$$\frac{1}{\varepsilon}\left[\left(\frac{H^{n+1/2}_{y,(i+\frac{1}{2},j)} - H^{n+1/2}_{y,(i-\frac{1}{2})}}{\Delta x}\right) - \left(\frac{H^{n+1/2}_{x,(i,j+\frac{1}{2})} - H^{n+1/2}_{x,(i,j-\frac{1}{2})}}{\Delta y}\right)\right]$$



Time eigenvalue problem

Introduce the generic vector component

$$\frac{V_{(i,j)}^{n+1/2} - V_{(i,j)}^{n-1/2}}{\Delta t} = \Lambda V_{(i,j)}^{n}$$



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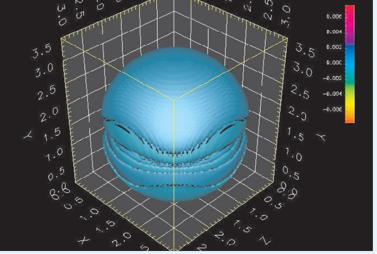
$$\frac{V_{(i,j)}^{n+1/2} - V_{(i,j)}^{n-1/2}}{\Delta t} = \Lambda V_{(i,j)}^{n}$$

and define a *solution growth factor*

$$q_{i,j} = \frac{V_{(i,j)}^{n+1/2}}{V_{(i,j)}^{n}} = \frac{V_{(i,j)}^{n}}{V_{(i,j)}^{n-1/2}}$$

for all n.



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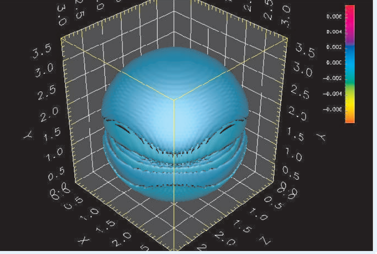
for all n.

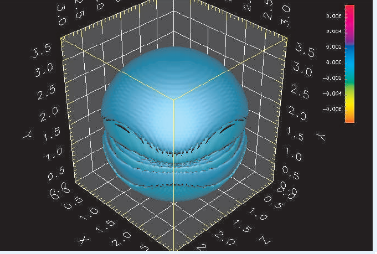
The goal: $|q_{i,j}| \leq 1$ to avoid uncontrolled growth and blow-up for all points (i, j).



Condition of temporal stability

After substitution and excluding $V^n_{(i,j)}$:

$$q^2_{i,j} - \Lambda \Delta t q_{i,j} - 1 = 0$$



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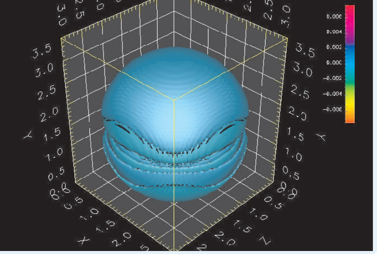
The solution:

$$q_{i,j} = \frac{\Lambda\Delta t}{2} + \sqrt{\left(\frac{\Lambda\Delta t}{2}\right)^2 + 1} = \alpha + \sqrt{\alpha^1 + 1}$$



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After substitution and excluding $V_{(i,j)}^{n}$:

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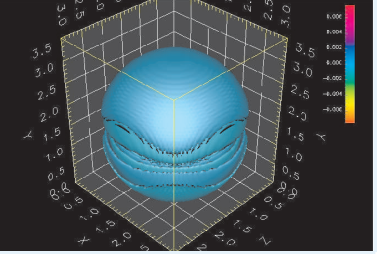
$|q_{i,j}| = 1$ **always** if $Re[\alpha] = 0$ and $-1 \leq Im[\alpha] \leq 1$; hence $\alpha = i \cdot Im[\alpha]$ and $\Lambda = i \cdot Im[\Lambda]$.



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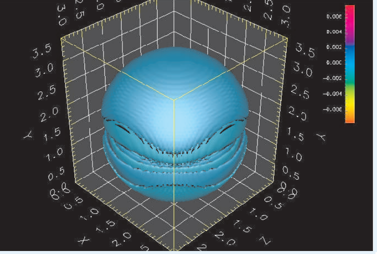
In this case

$$-1 \leq \frac{Im[\Lambda]\Delta t}{2} \leq 1 \Rightarrow -\frac{2}{\Delta t} \leq Im[\Lambda] \leq \frac{2}{\Delta t}$$



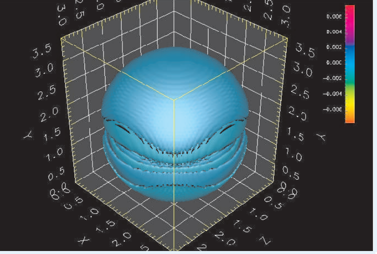
Space eigenvalue problem

We isolate space differentiation operation:

$$-\frac{1}{\mu}\left(\frac{E_{z,(i,j+\frac{1}{2})}-E_{z,(i,j-\frac{1}{2})}}{\Delta y}\right)=\Lambda H_{x,(i,j)}$$

$$\frac{1}{\mu}\left(\frac{E_{z,(i+\frac{1}{2},j)}-E_{z,(i-\frac{1}{2},j)}}{\Delta x}\right)=\Lambda H_{y,(i,j)}$$

$$\frac{1}{\varepsilon}\left[\left(\frac{H_{y,(i+\frac{1}{2},j)}-H_{y,(i-\frac{1}{2})}}{\Delta x}\right)-\left(\frac{H_{x,(i,j+\frac{1}{2})}-H_{x,(i,j-\frac{1}{2})}}{\Delta y}\right)\right]=\Lambda E_{z,(i,j)}$$



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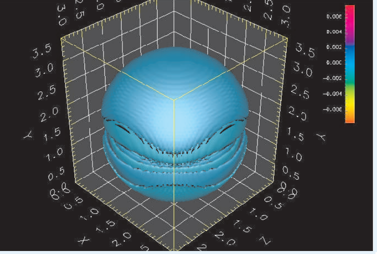
$$\frac{1}{\varepsilon}\left[\left(\frac{H_{y,(i+\frac{1}{2},j)}-H_{y,(i-\frac{1}{2})}}{\Delta x}\right)-\left(\frac{H_{x,(i,j+\frac{1}{2})}-H_{x,(i,j-\frac{1}{2})}}{\Delta y}\right)\right]=\Lambda E_{z,(i,j)}$$

and look for solution in form of the *plane wave* with $\tilde{k}_x$ and $\tilde{k}_y$ are the components of wave-vector in x and y directions:

$$E_{z,(I,J)}=E_{z_0}\exp[i(\tilde{k}_x I\Delta x+\tilde{k}_y J\Delta y)]$$

$$E_{x,(I,J)}=H_{x_0}\exp[i(\tilde{k}_x I\Delta x+\tilde{k}_y J\Delta y)]$$

$$E_{y,(I,J)}=H_{y_0}\exp[i(\tilde{k}_x I\Delta x+\tilde{k}_y J\Delta y)]$$

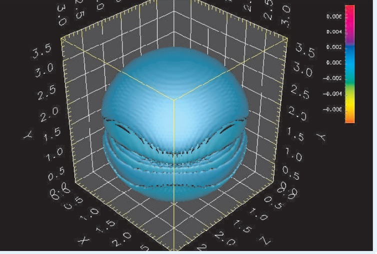


Condition of spatial stability

After substitution and applying *Euler's Identity*:

$$H_{x_0} = \frac{2iE_{z_0}}{\lambda\mu\Delta y}\sin\left(\frac{\tilde{k}_y\Delta y}{2}\right), \quad H_{y_0} = \frac{2iE_{z_0}}{\lambda\mu\Delta x}\sin\left(\frac{\tilde{k}_x\Delta x}{2}\right)$$

$$E_{z_0} = \frac{2i}{\Lambda\varepsilon}\left[\frac{2iH_{y_0}}{\Delta x}\sin\left(\frac{\tilde{k}_x\Delta x}{2}\right) - \frac{2iH_{x_0}}{\Delta y}\sin\left(\frac{\tilde{k}_y\Delta y}{2}\right)\right]$$



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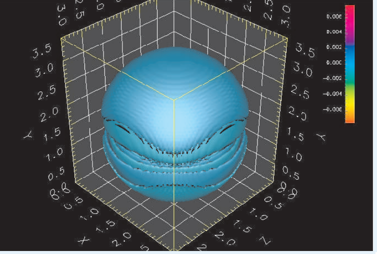
After substituting H_{x_0} and H_{y_0} and eliminating E_{z_0} we obtain:

$$\Lambda^2 = -\frac{4}{\mu\varepsilon}\left[\frac{1}{(\Delta x)^2}\sin^2\left(\frac{\tilde{k}_x\Delta x}{2}\right) + \frac{1}{(\Delta y)^2}\sin^2\left(\frac{\tilde{k}_y\Delta y}{2}\right)\right]$$



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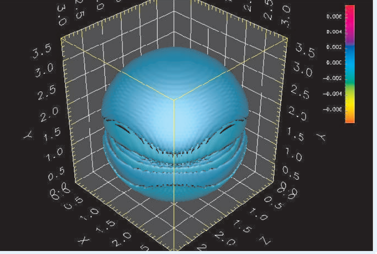
Using the fact that $Re[\Lambda] = 0$ and the bounds of $\sin(.)$ we write:

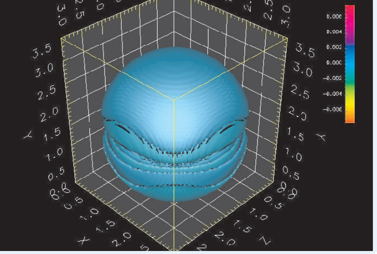
$$-2c\sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}} \leq Im[\Lambda] \leq 2c\sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}},$$

where $c = 1\sqrt{\varepsilon\mu}$ is a speed of light.



Enforcing stability of Yee algorithm

$$2c\sqrt{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}} \leq \frac{2}{\Delta t} \Rightarrow \Delta t \leq \frac{1}{c\sqrt{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}}}$$



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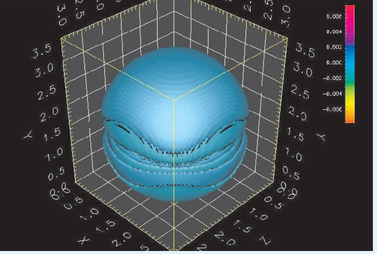
When $\Delta x = \Delta y = \Delta$:

$$\Delta t = \frac{\Delta}{c\sqrt{2}}$$



Enforcing stability of Yee algorithm

$$2c\sqrt{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}} \leq \frac{2}{\Delta t} \Rightarrow \Delta t \leq \frac{1}{c\sqrt{\frac{1}{(\Delta x)^2}+\frac{1}{(\Delta y)^2}}}$$

When $\Delta x = \Delta y = \Delta$:

$$\Delta t = \frac{\Delta}{c\sqrt{2}}$$

In practical applications, we always intend to keep Δt *as large as possible to minimize the computational time, but its value should be always less (at least slightly) than the upper bound to avoid instability caused by the "numerical junk" accumulation*.