Universidad de Oviedo

Grado en Física

Métodos Numéricos
y sus
Aplicaciones a la Física

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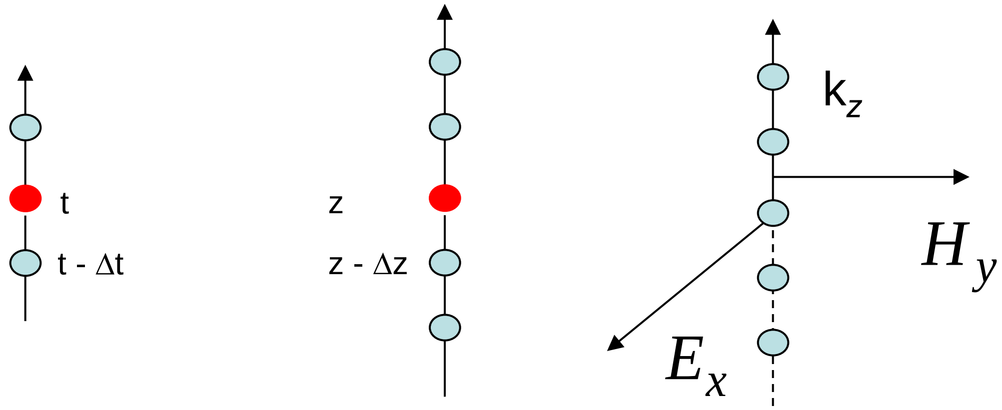
Diferencias Finitas en el dominio del tiempo

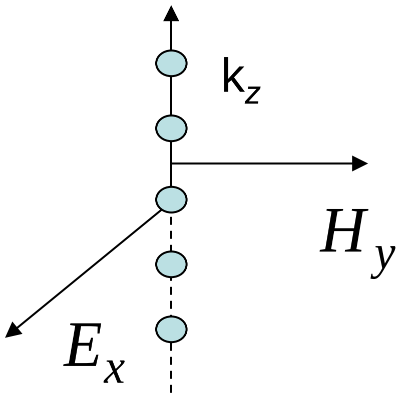
FDTD

$$\mu_0 \frac{\partial \vec{H}}{\partial t} = -\left(\nabla \times \vec{E}\right) \qquad \varepsilon \frac{\partial \vec{E}}{\partial t} = \left(\nabla \times \vec{H}\right) - \vec{J}_{ex}$$

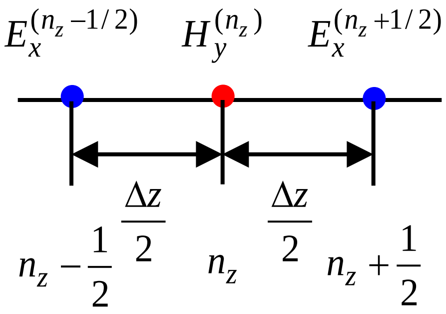


$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_o}\frac{\partial E_x}{\partial z} \qquad \varepsilon \frac{\partial E_x}{\partial t} = \frac{\partial H_y}{\partial z} - J_{ex}$$

1 - D

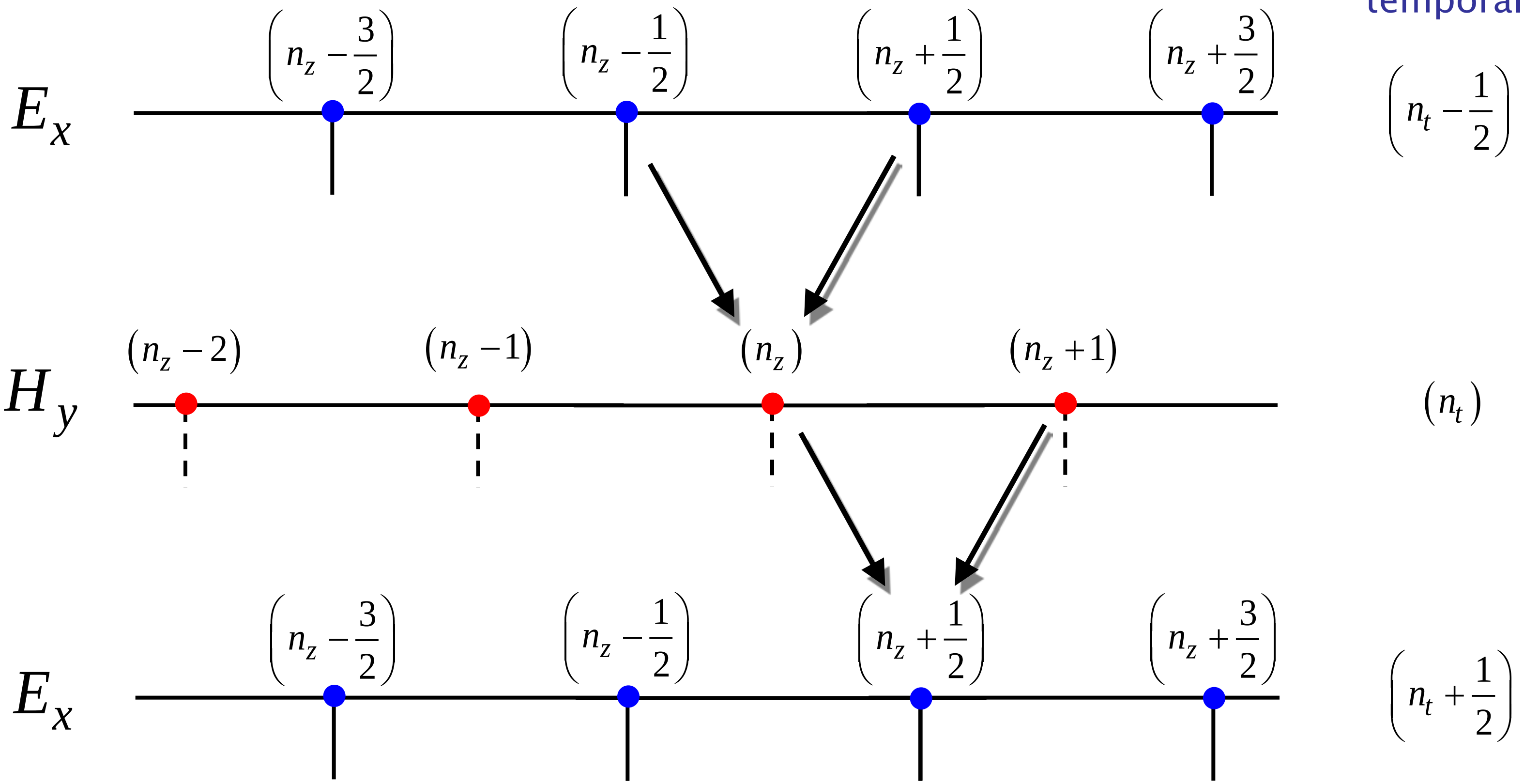


Mallado espacial “Staggered”
“escalonado”

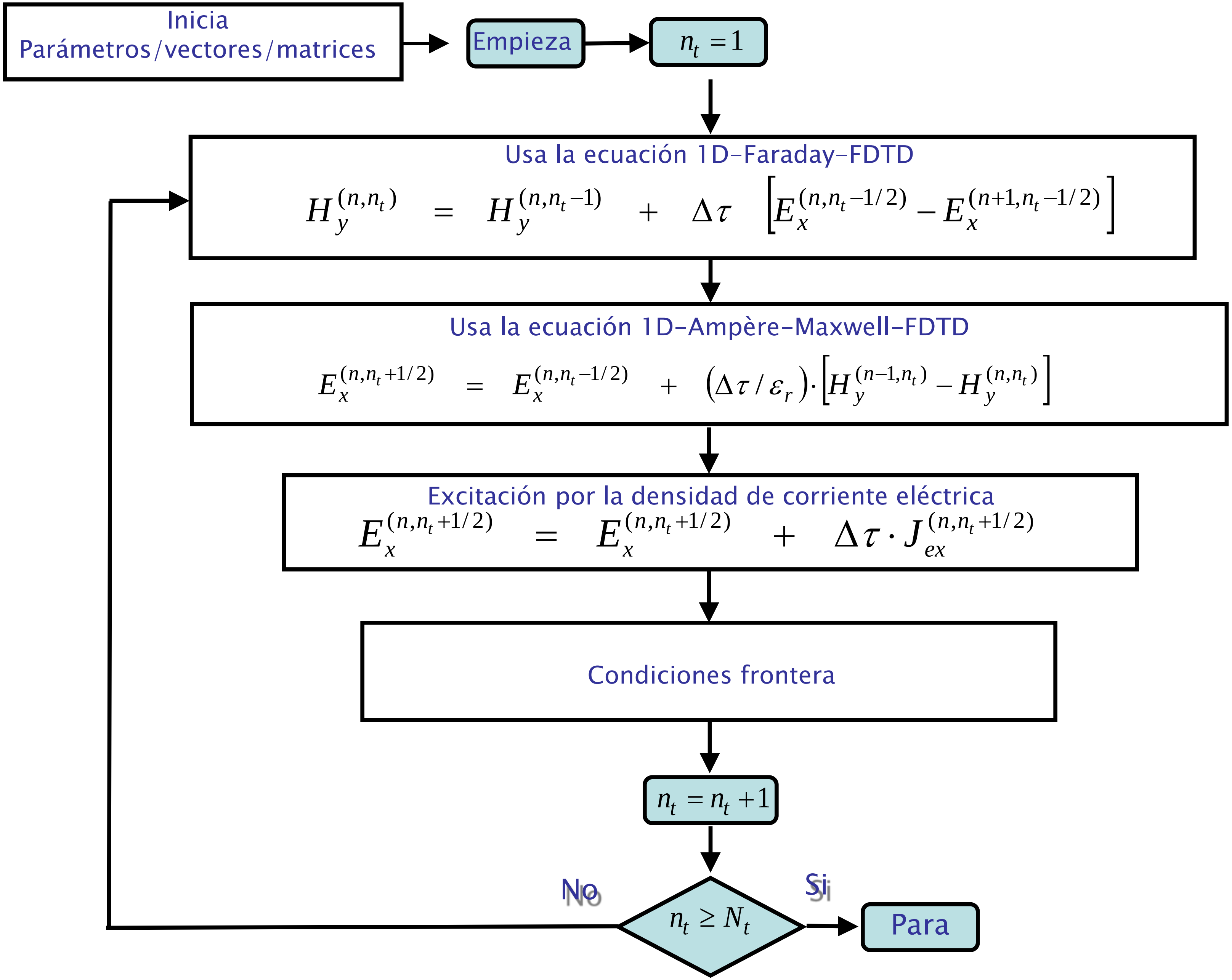


Algorítmo temporal tipo “Leap-frog”
“salto de rana”

Plano temporal



1-D Algoritmo FDTD / Diagrama de flujo



Inicia
Parámetros/vectores/matrices

Empieza

$n_t = 1$

Usa la ecuación 1D-Faraday-FDTD

$$H_y^{(n,n_t)} = H_y^{(n,n_t-1)} + \Delta\tau \left[E_x^{(n,n_t-1/2)} - E_x^{(n+1,n_t-1/2)}\right]$$

Usa la ecuación 1D-Ampère-Maxwell-FDTD

$$E_x^{(n,n_t+1/2)} = E_x^{(n,n_t-1/2)} + (\Delta\tau/\varepsilon_r)\cdot\left[H_y^{(n-1,n_t)} - H_y^{(n,n_t)}\right]$$

Excitación por la densidad de corriente eléctrica

$$E_x^{(n,n_t+1/2)} = E_x^{(n,n_t+1/2)} + \Delta\tau \cdot J_{ex}^{(n,n_t+1/2)}$$

Condiciones frontera

$n_t = n_t + 1$

$n_t \geq N_t$

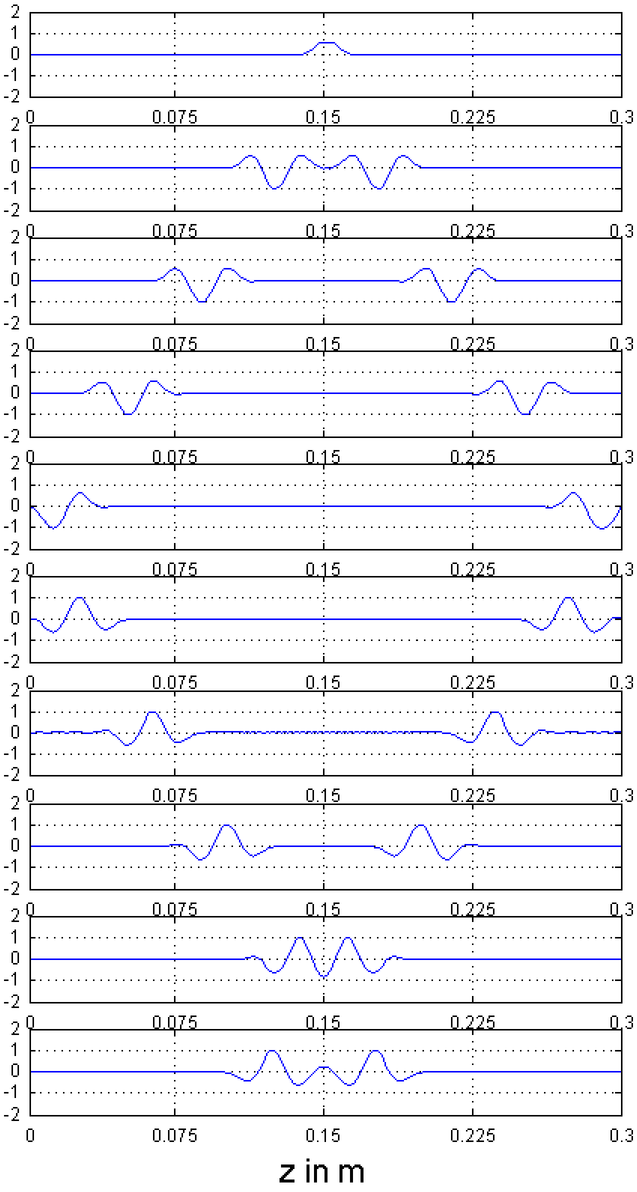
No

Si

Para

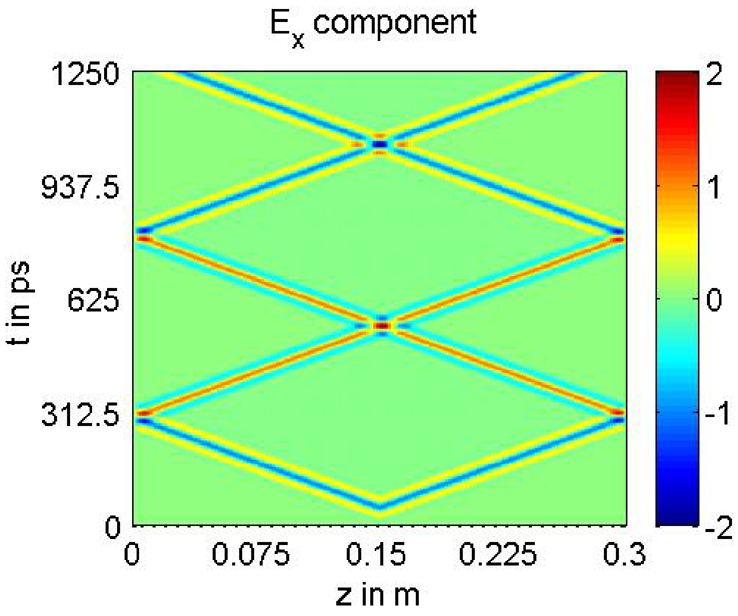
Condiciones frontera

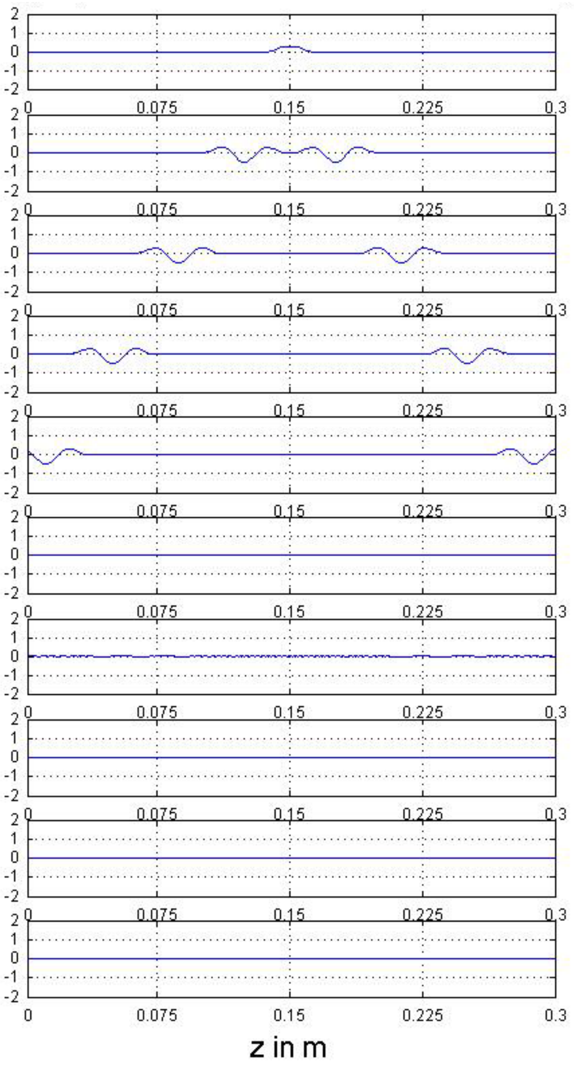
$E_x(z,t_0)$ a distintos t_0

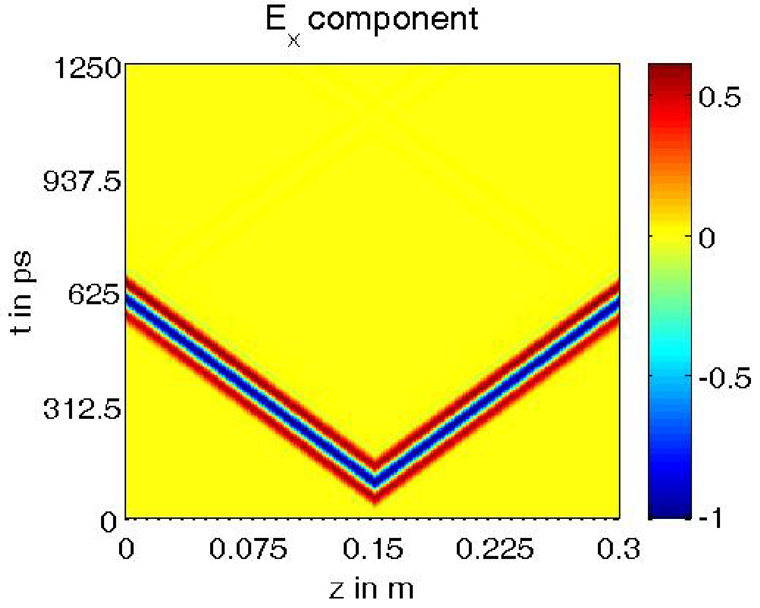


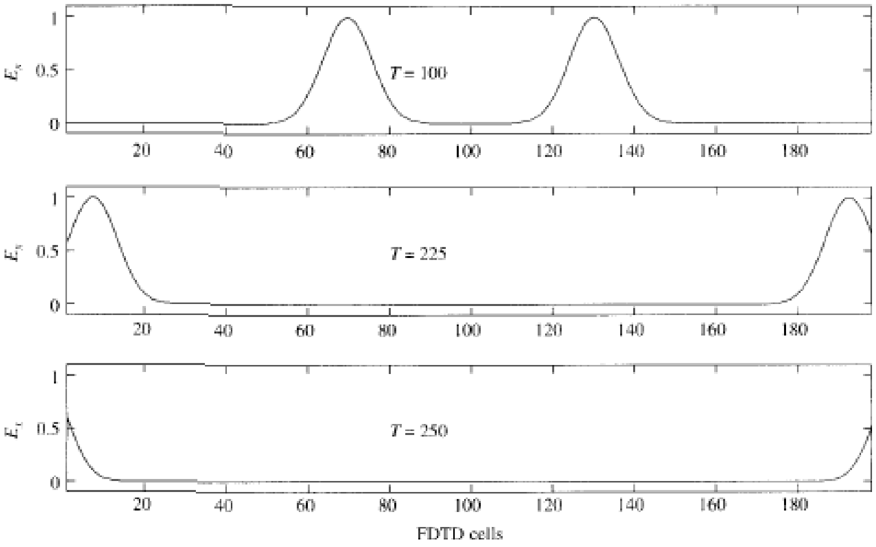
$$\left.\begin{array}{r} E_x^{(1,n_t)} = 0 \\ E_x^{(N_z,n_t)} = 0 \end{array}\right\} \quad 1 \le n_t \le N_t$$

Condiciones frontera no válidas





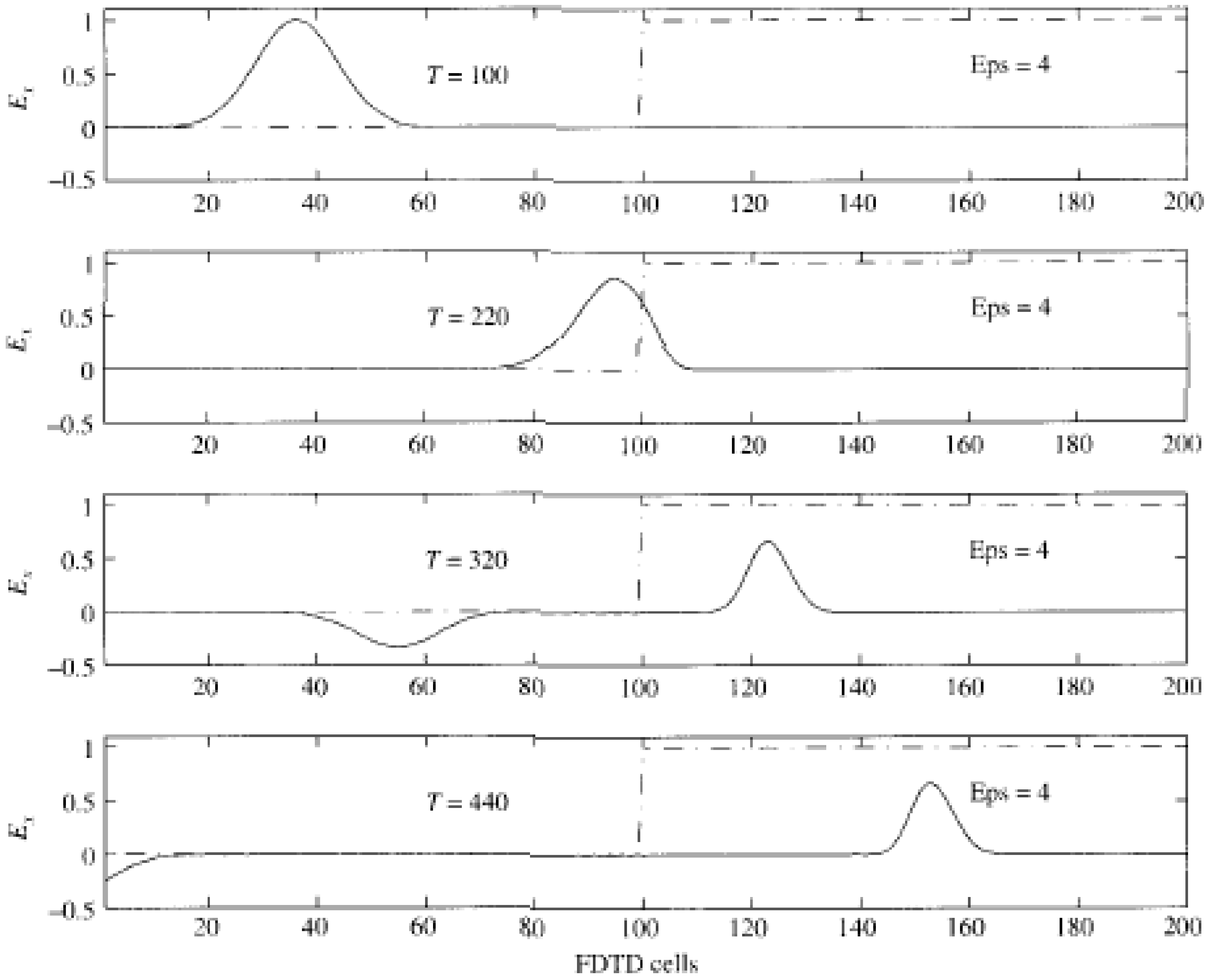




Si $c\Delta t = \Delta z/2$ una onda plana necesita dos pasos de tiempo, $2n_t$, para viajar a través de una celda de espaciado Δz

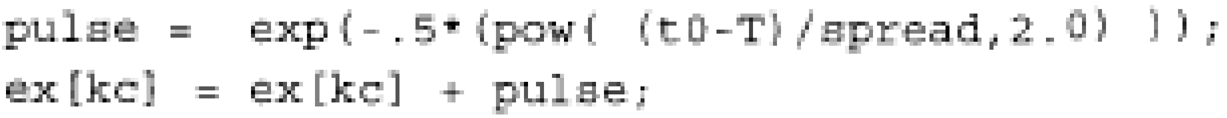
$$\left.\begin{array}{l} E_x^{(1,n_t)} = E_x^{(2,n_t-2)} \\ E_x^{(N_z,n_t)} = E_x^{(N_z-1,n_t-2)} \end{array}\right\} \quad 1 \le n_t \le N_t$$

¡ Guarda $E_x(2)$, $E_x(N-1)$ para dos tiempos y almacénalo en $E_x(1)$, $E_x(N)$!



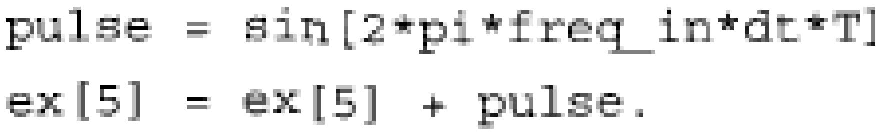
E_x
1
0.5
0
−0.5
T = 100
T = 220
T = 320
T = 440
Eps = 4
20
40
60
80
100
120
140
160
180
200
FDTD cells

Tipos de fuentes blandas



```
pulse =  exp(-.5*(pow( (t0-T)/spread,2.0) ));
ex[kc] = ex[kc] + pulse;
```

Gausiana

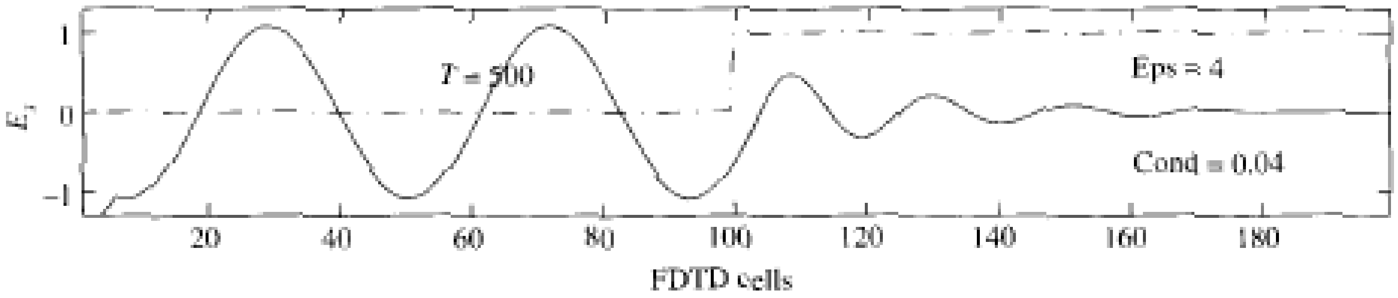


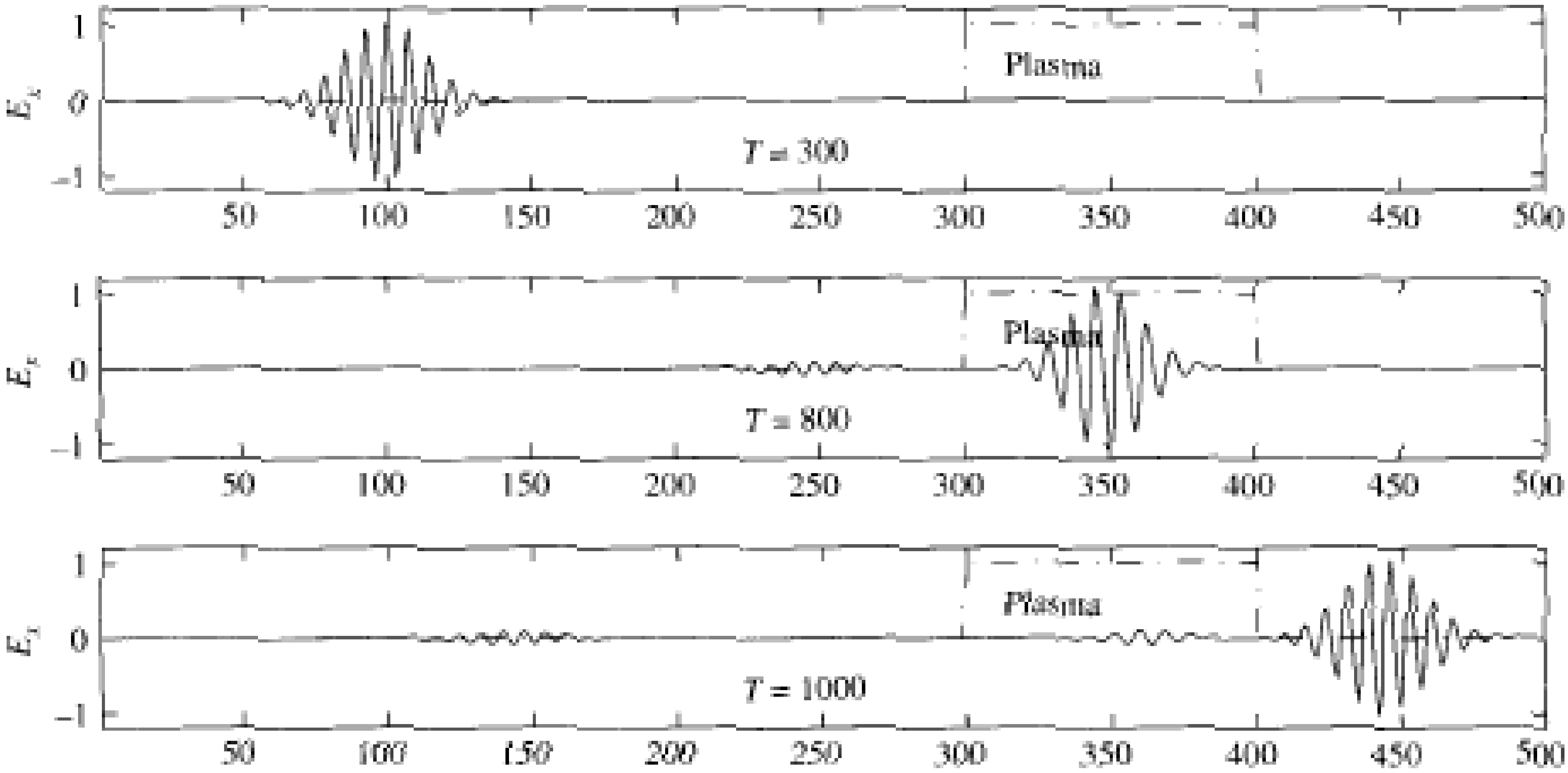
```
pulse = sin[2*pi*freq_in*dt*T]
ex[5] = ex[5] + pulse.
```

Sinusoidal

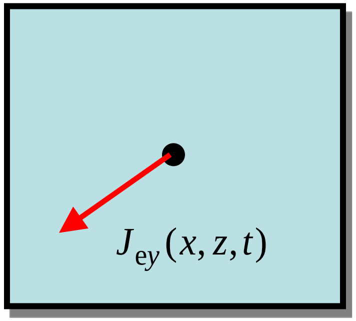
Anchura de la celda

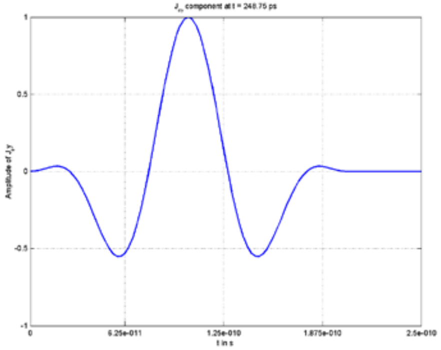
Para una buena resolución espacial
$\Delta x = \lambda /10$

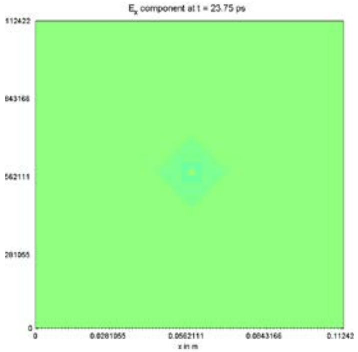


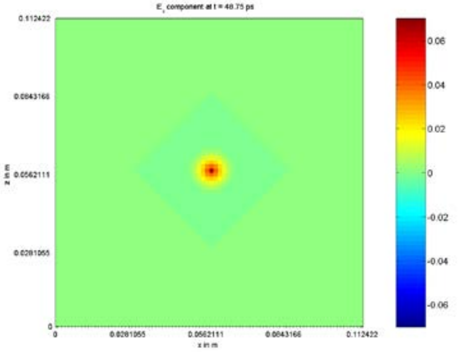


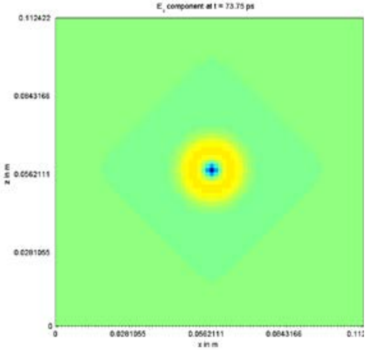
E_y
1
0
−1
Plasma
$T = 300$
$T = 800$
$T = 1000$
50
100
150
200
250
300
350
400
450
500

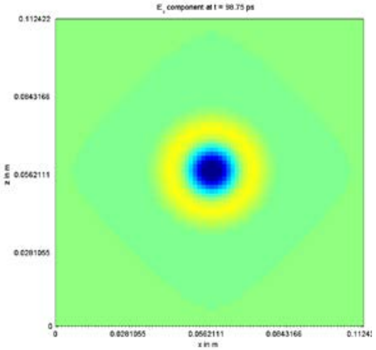

$J_{ey}(x,z,t)$

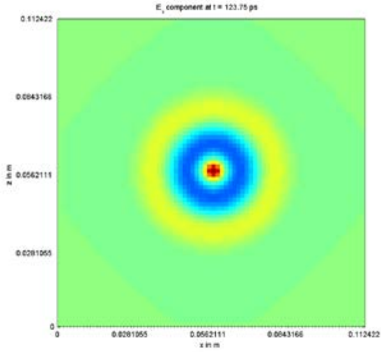

J_{ey} component at t = 248.75 ps
Amplitude of J_y
1
0.5
0
-0.5
-1
0
6.25e-011
1.25e-010
1.875e-010
2.5e-010
t in s

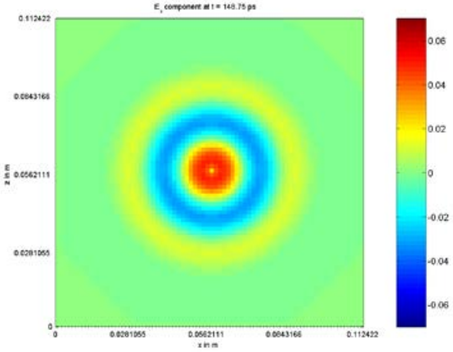

E_x component at t = 23.75 ps
112422
843166
562111
281055
0
0
0.0281055
0.0562111
0.0843166
0.11242
x in m

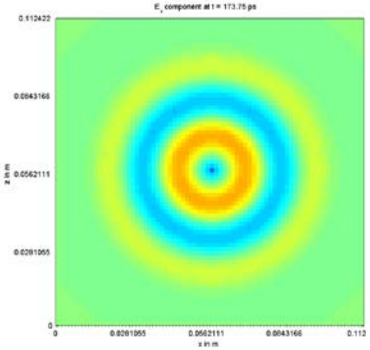

E_y component at t = 48.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.112422
x in m
0.06
0.04
0.02
0
-0.02
-0.04
-0.06

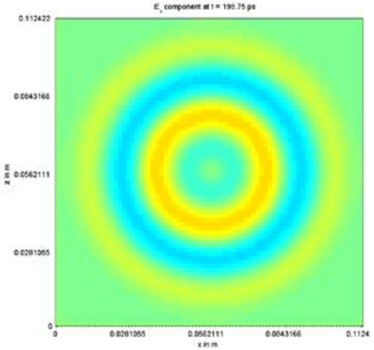

E_y component at t = 73.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.112
x in m

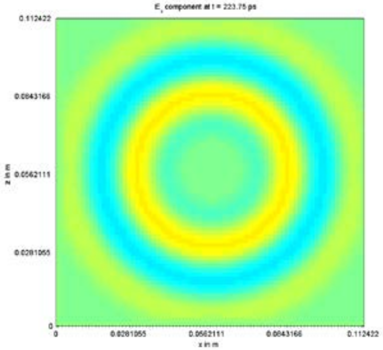

E_y component at t = 98.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.1124
x in m

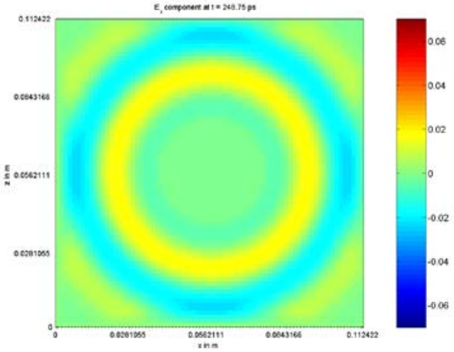

E_y component at t = 123.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.112422
x in m


E_y component at t = 148.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.112422
x in m
0.06
0.04
0.02
0
-0.02
-0.04
-0.06

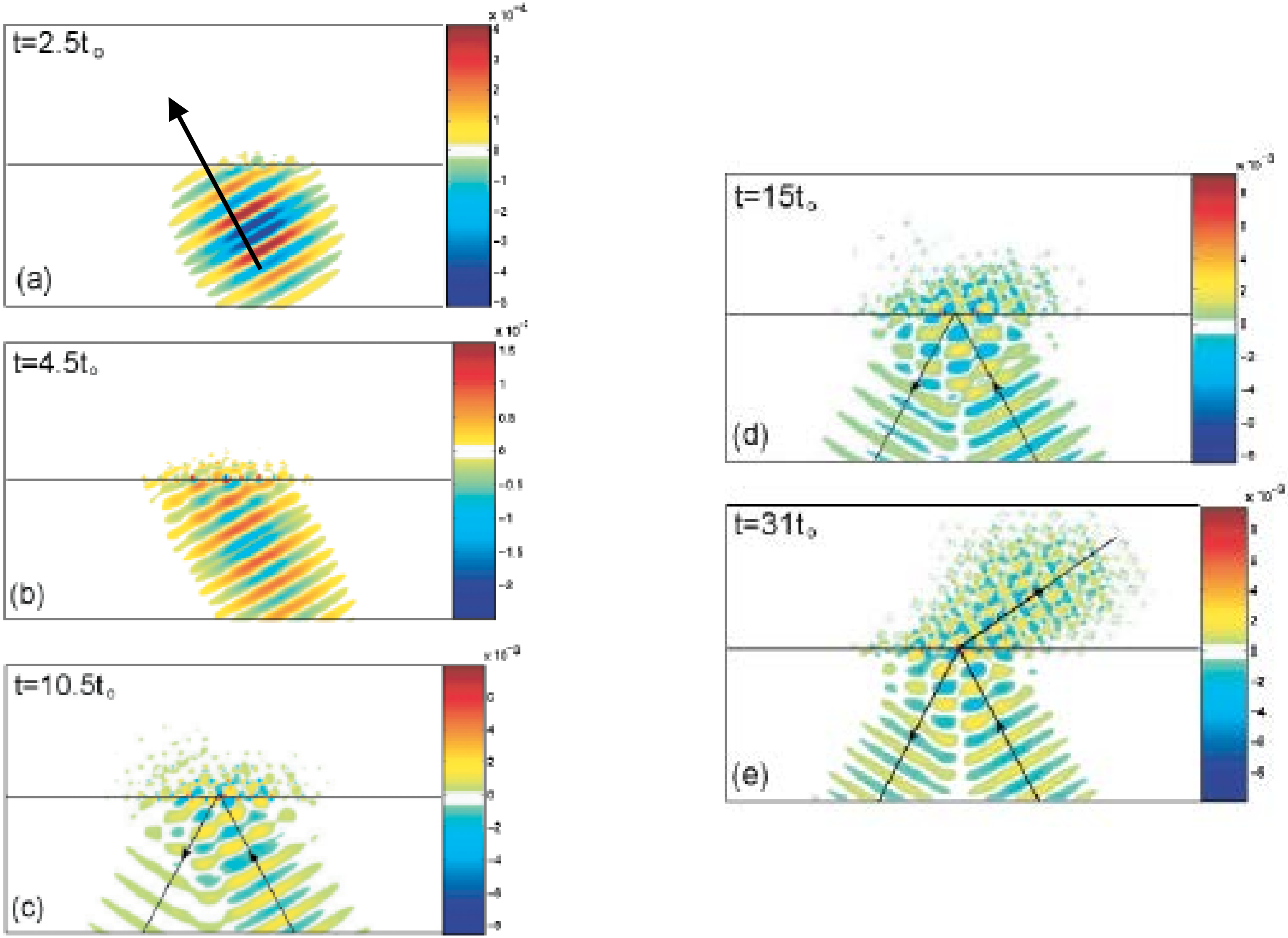

E_y component at t = 173.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.112
x in m


E_y component at t = 198.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.1124
x in m

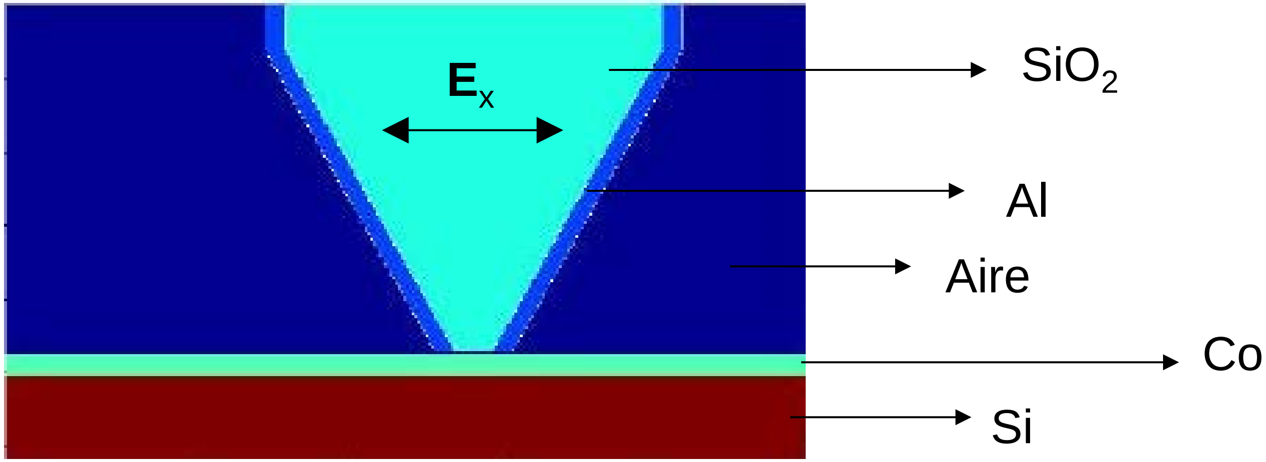

E_y component at t = 223.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.112422
x in m


E_y component at t = 248.75 ps
z in m
0.112422
0.0843166
0.0562111
0.0281055
0
0
0.0281055
0.0562111
0.0843166
0.112422
x in m
0.06
0.04
0.02
0
-0.02
-0.04
-0.06

Refraction in Media with a Negative Refractive Index

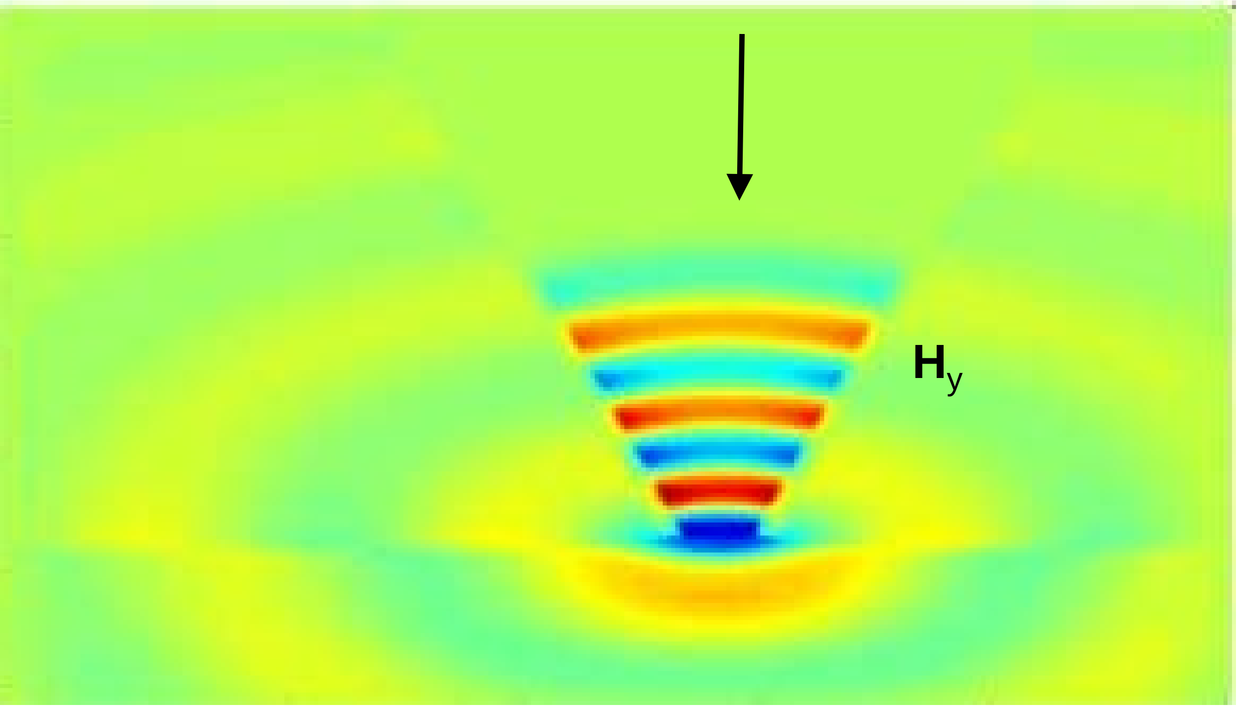


Co(60nm)/Si



λ = 633 nm
abertura = 96 nm
$d_{punta-muestra}$ = 20 nm

1100x1100 celdas^2
Área celda= 2x2 nm^2



Evolución temporal de una función de onda

Método explícito (FDTD)

$$\boxed{i\hbar\frac{\partial\psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V(r,t)\cdot\psi(r,t)}$$

$$\frac{\partial\psi(r,t)}{\partial t} = i\frac{\hbar}{2m}\nabla^2\psi(r,t) - \frac{i}{\hbar}V(r,t)\cdot\psi(r,t),$$

$$\psi(r,t) = \psi_{\mathrm{real}}(r,t) + i\,\psi_{\mathrm{imag}}(r,t). \quad \begin{cases} \dfrac{\partial\psi_{\mathrm{real}}(r,t)}{\partial t} = -\dfrac{\hbar}{2m}\cdot\nabla^2\psi_{\mathrm{imag}}(r,t) + \dfrac{1}{\hbar}V\,\psi_{\mathrm{imag}}(r,t) & [\ 1\ ] \\[2ex] \dfrac{\partial\psi_{\mathrm{imag}}(r,t)}{\partial t} = \dfrac{\hbar}{2m}\cdot\nabla^2\psi_{\mathrm{real}}(r,t) - \dfrac{1}{\hbar}V\,\psi_{\mathrm{real}}(r,t). & [\ 2\ ] \end{cases}$$

$$\frac{\psi^{n}_{\mathrm{real}}(k) - \psi^{n-1}_{\mathrm{real}}(k)}{\Delta t} = -\frac{\hbar}{2m}\,\frac{\psi^{n-1/2}_{\mathrm{imag}}(k+1) - 2\psi^{n-1/2}_{\mathrm{imag}}(k) + \psi^{n-1/2}_{\mathrm{imag}}(k-1)}{(\Delta z)^2} + \frac{1}{\hbar}V(k)\cdot\psi^{n-1/2}_{\mathrm{imag}}(k). \quad [\ 1\ ]$$

Método semi-implícito (Crank-Nicolson)

Am. J. Phys. 50, 902 (1982);

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t).$$

$a\equiv i\hbar$ $b= -a^2/2m$

$$\frac{b}{(\Delta x)^2}\Psi(x_{i+1},t_j)+\overbrace{\left(\frac{2a}{\Delta t}-\frac{2b}{(\Delta x)^2}-V(x_i)\right)}^{\alpha_i}\Psi(x_i,t_j)+\frac{b}{(\Delta x)^2}\Psi(x_{i-1},t_j)+b\left[\Psi(x_{i+1},t_{j-1})-2\Psi(x_i,t_{j-1})+\Psi(x_{i+1},t_{j-1})\right]$$

$$=\left(\frac{2a}{\Delta t}+V(x_i)\right)\Psi(x_i,t_{j-1})$$

$$\begin{pmatrix} 1 & 0 & 0 & & & \\ 0 & \alpha_1 & \frac{b}{(\Delta x)^2} & & & \\ 0 & \frac{b}{(\Delta x)^2} & \alpha_2 & & & \\ & & & \alpha_{n-2} & \frac{b}{\Delta x^2} & 0 \\ & & & \frac{b}{\Delta x^2} & \alpha_{n-1} & \frac{b}{\Delta x^2} \\ & & & & 0 & 1 \end{pmatrix} \times \begin{pmatrix} \Psi(x_0,t_j) \\ \Psi(x_1,t_j) \\ \Psi(x_2,t_j) \\ \Psi(x_{n-2},t_j) \\ \Psi(x_{n-1},t_j) \\ \Psi(x_n,t_j) \end{pmatrix} = \begin{pmatrix} 0 \\ \beta_1 \\ \beta_2 \\ \beta_{n-2} \\ \beta_{n-1} \\ 0 \end{pmatrix}.$$