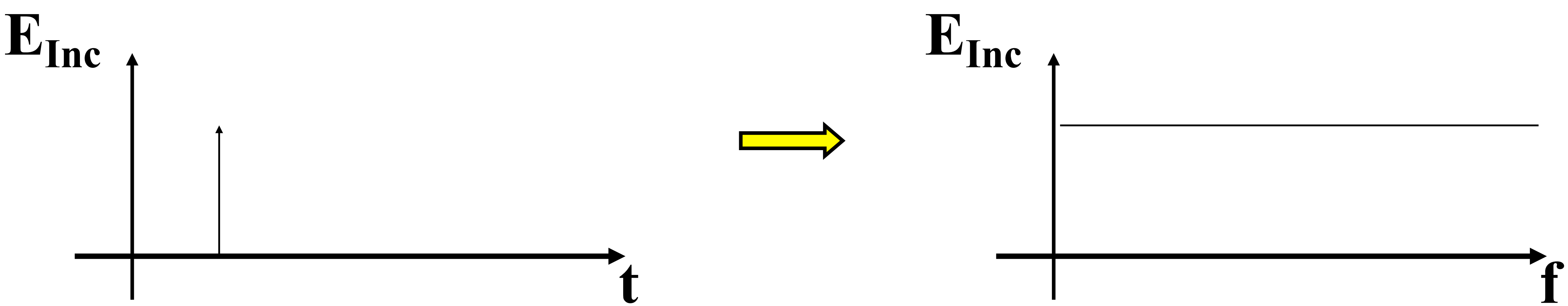
Computational Photonics

Finite-Difference Time-Domain

Relation between frequency and time domain

- the frequency spectrum used for the illumination is given by the Fourier-transformation of the time dependent incident field



- with a single calculation we can calculate the entire frequency response, detecting the temporal evolution of the field behind a structure and FT

(N_t = total number of time steps)

$$\Delta f = \frac{1}{T} = \frac{1}{N_t \cdot \Delta t}$$

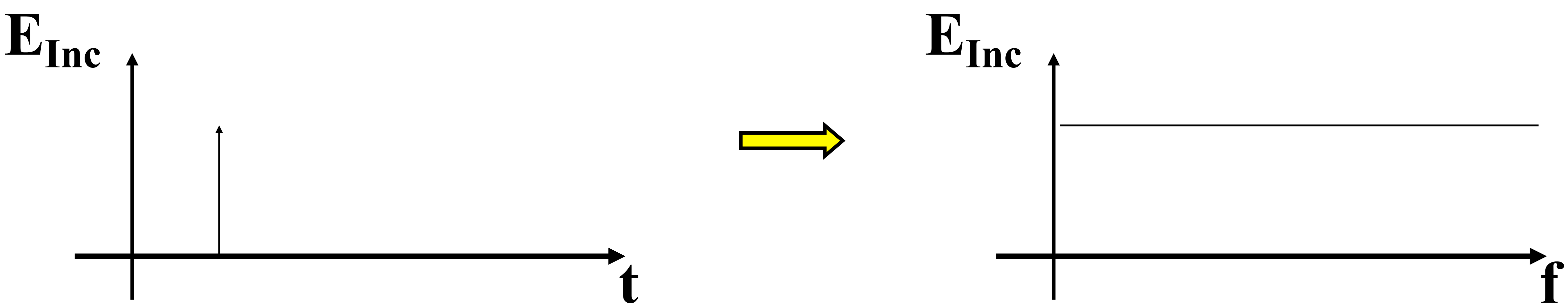
(frequency resolution)

$$\Delta\lambda = \frac{\lambda^2}{c \cdot \Delta t \cdot N_t}$$

(wavelength resolution)

Relation between frequency and time domain

- the frequency spectrum used for the illumination is given by the Fourier-transformation of the time dependent incident field

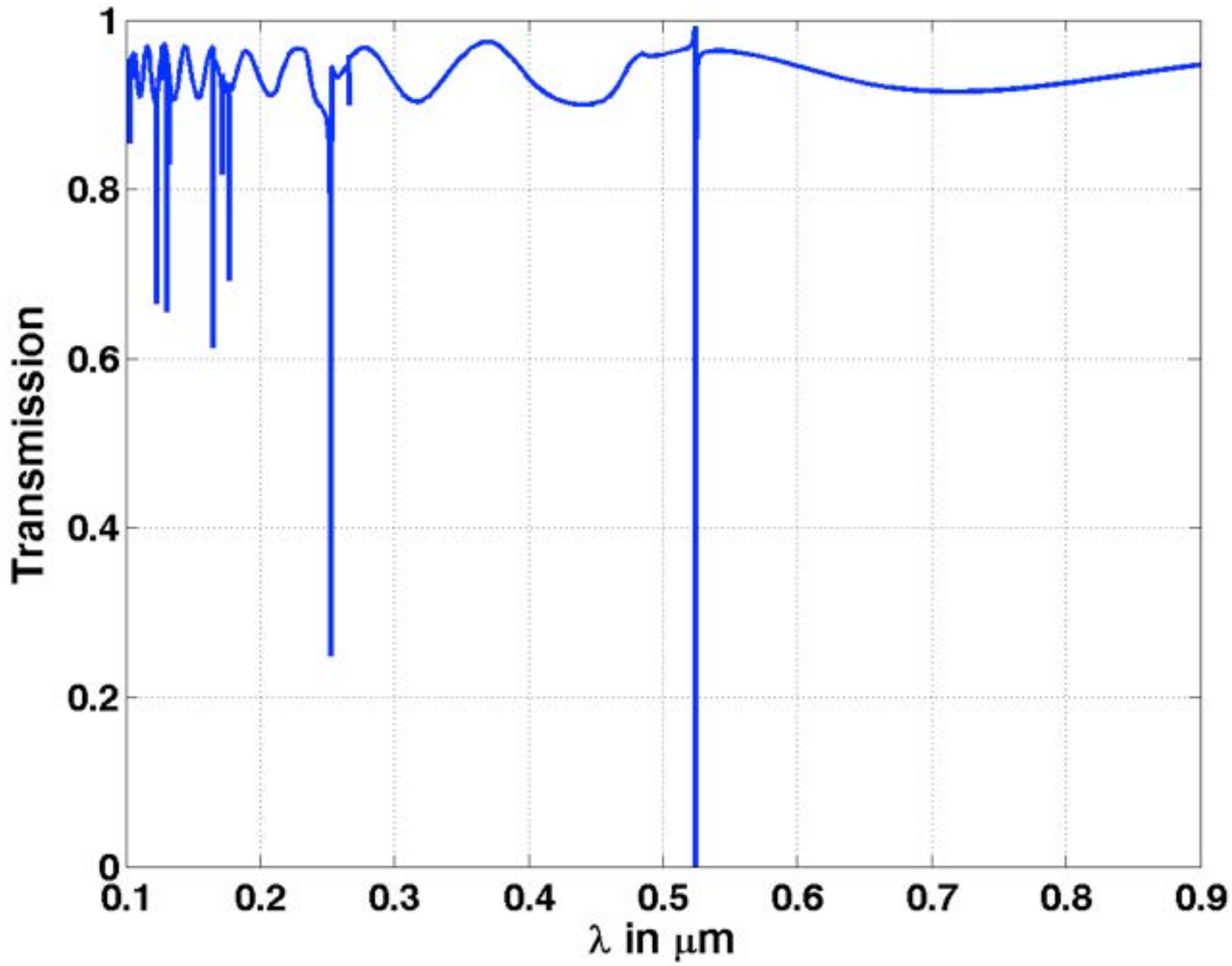


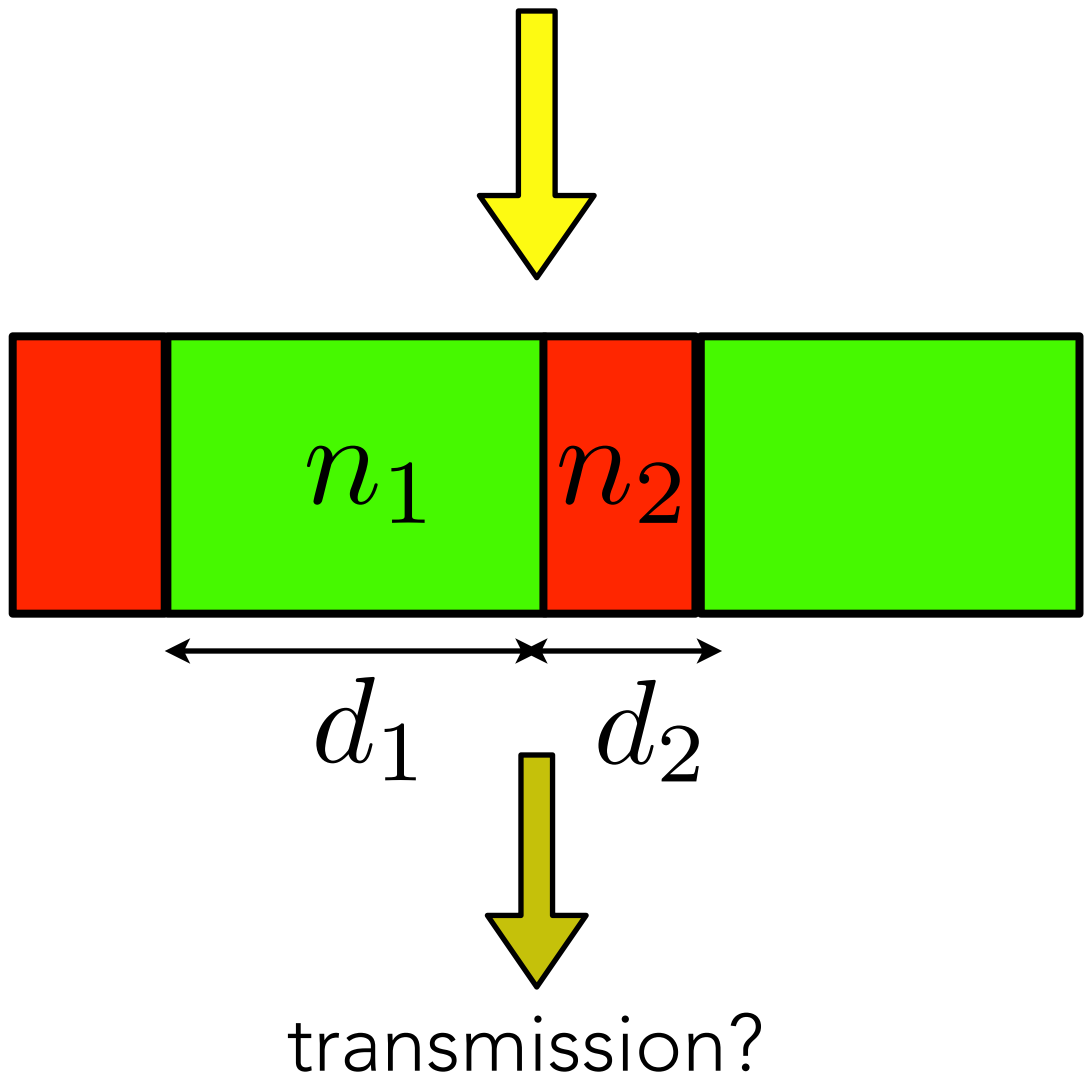
- with a single calculation we can calculate the entire frequency response, detecting the temporal evolution of the field behind a structure and FT (N_t = total number of time steps)

⇒ for a high resolution in the wavelength domain, we have to record the temporal evolution of the field for an excess in time

kind of disadvantage

Example of a grating wave guide coupler

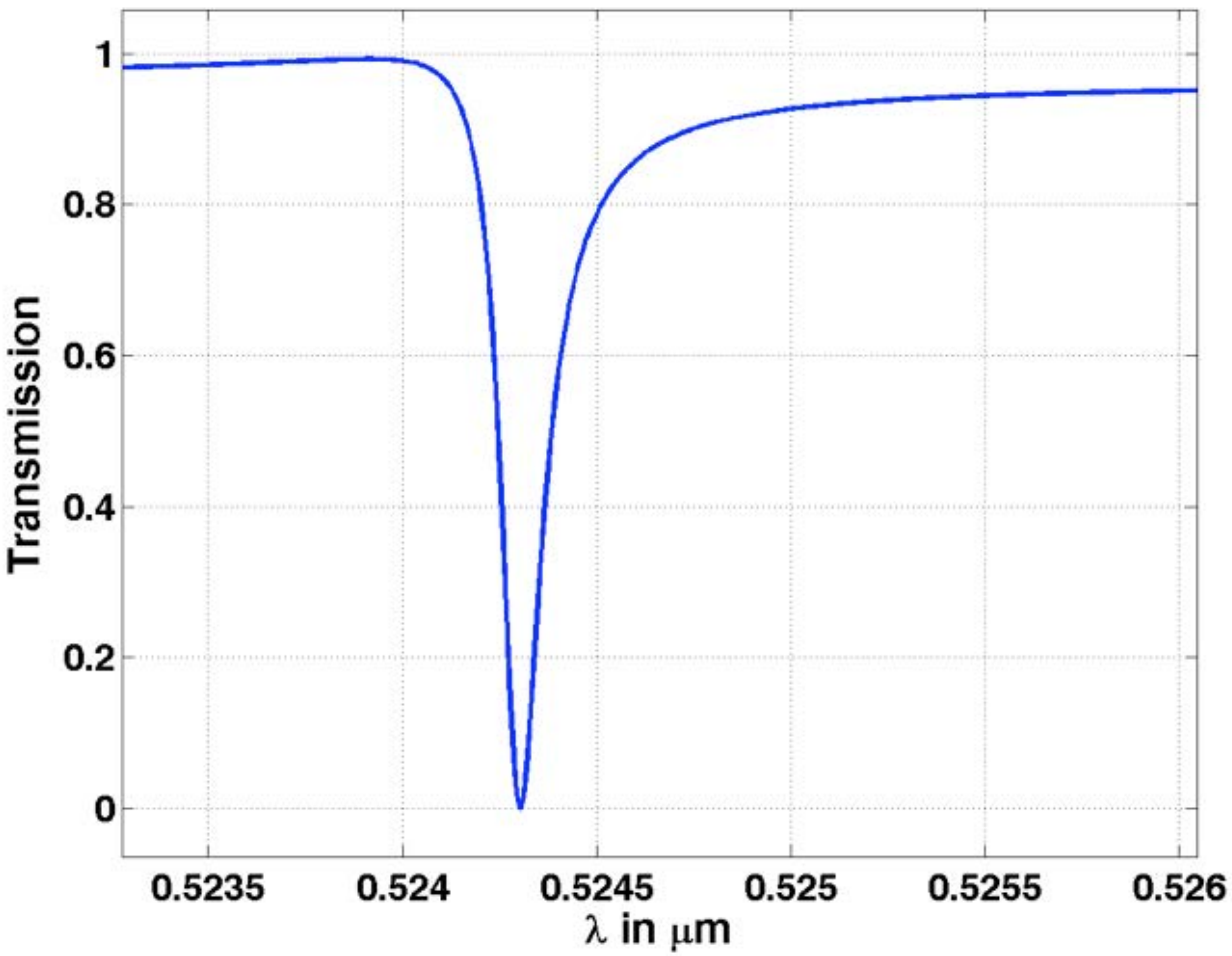


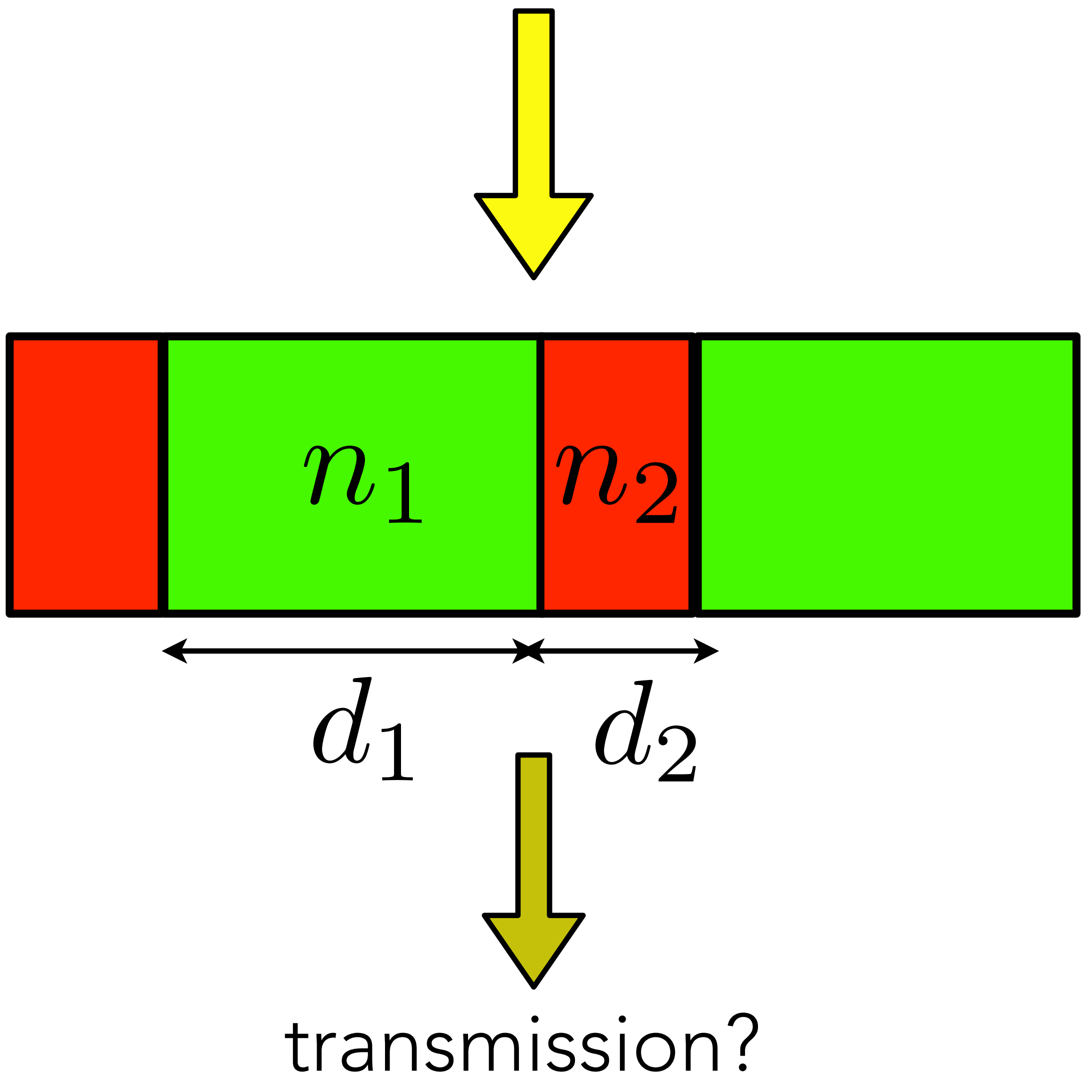


transmission function of a PC wave guide

(n1=1.58, n2=1.87,d1=d2=165nm, TE)

Example of a grating wave guide coupler





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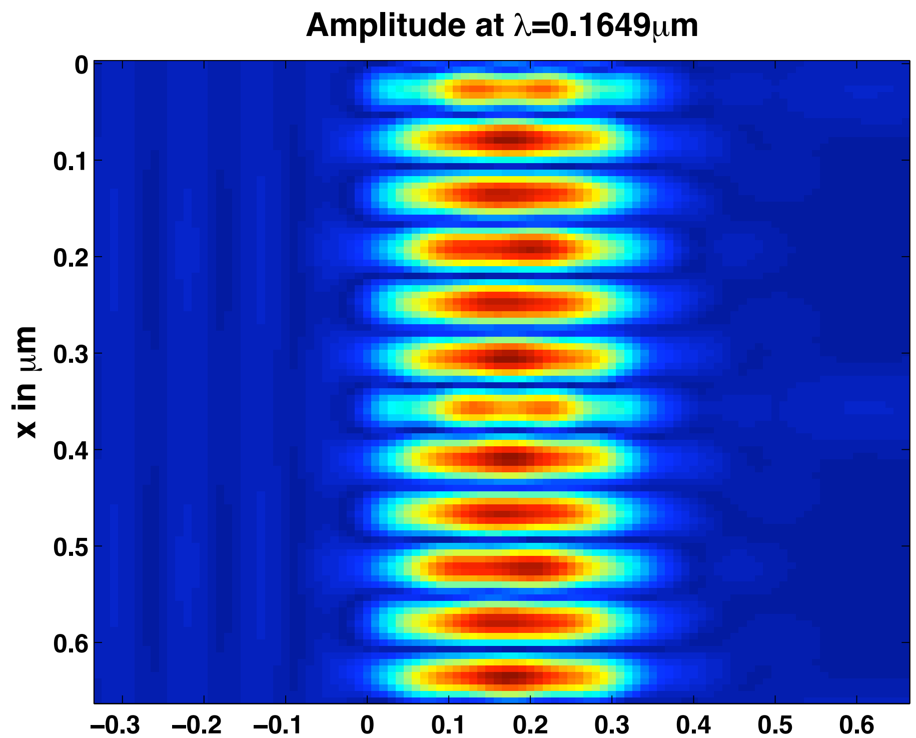
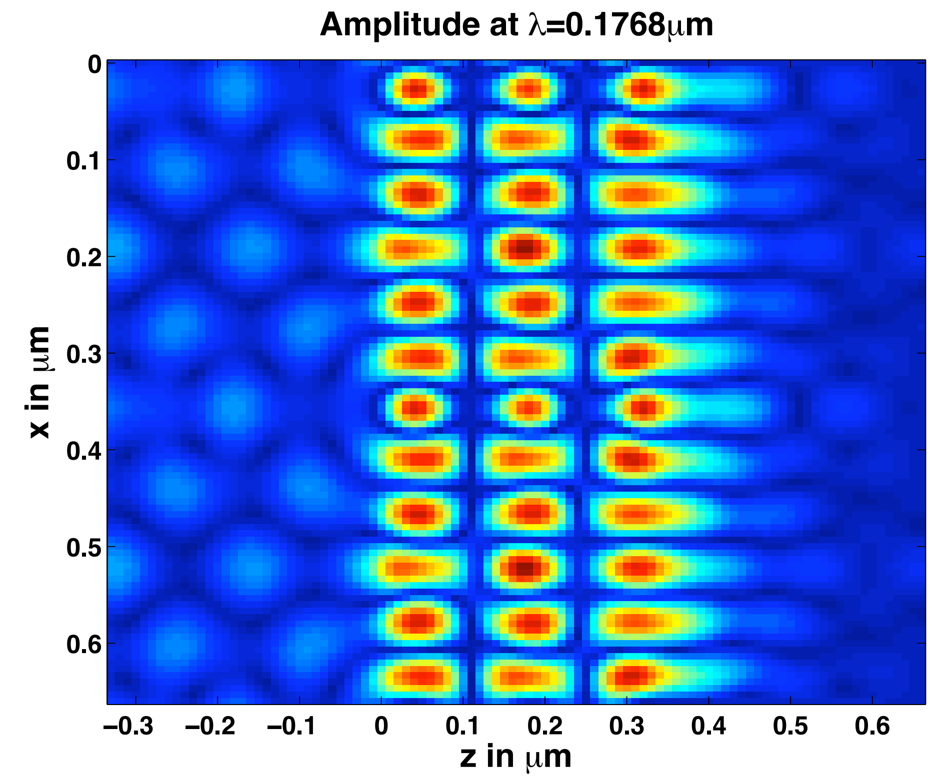
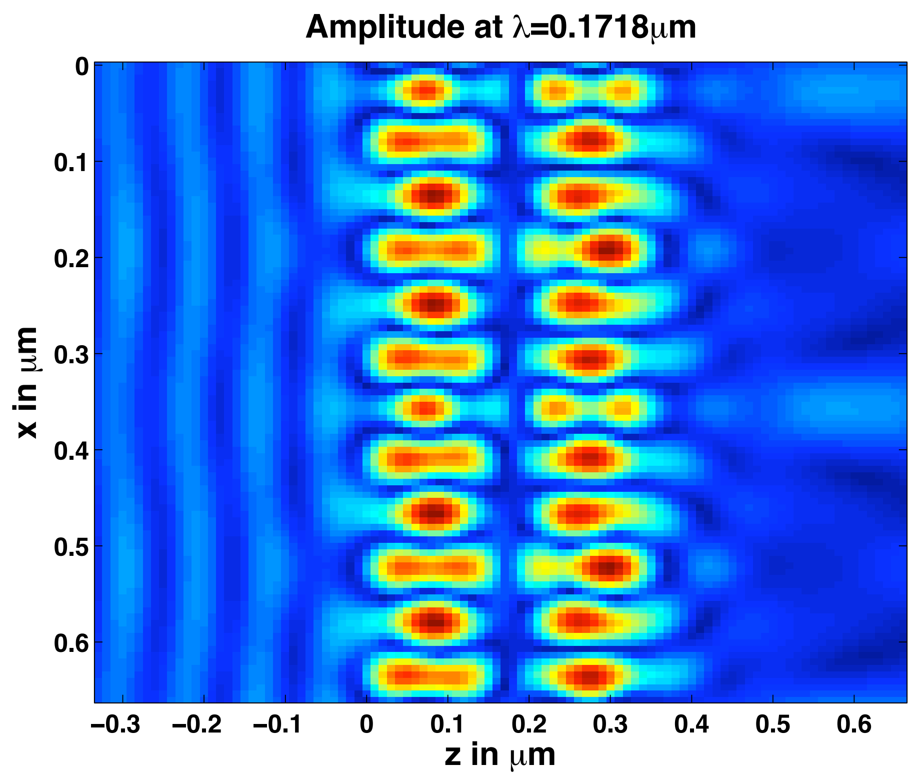
Example of a grating wave guide coupler







dips are waveguide resonances excited if the momentum provided by the grating matches the propagation constant of a waveguide mode

Inclusion of other materials

- FDTD is not directly applicable for materials with $\epsilon < 1$ (e.g. metals)
- material properties depend strongly on the wavelength (dispersion)
- nonlinear properties of interest (instantaneous or non-instantaneous)
- great diversity of approaches, but they require usually all the simulation of an additional quantity
- so far we have taken into account $\mathbf{E}$ and $\mathbf{H}$

$\Longrightarrow$ **J Current density** | **P Polarisation** | **D Displacement**

FDTD for metals

Maxwell:

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}$$

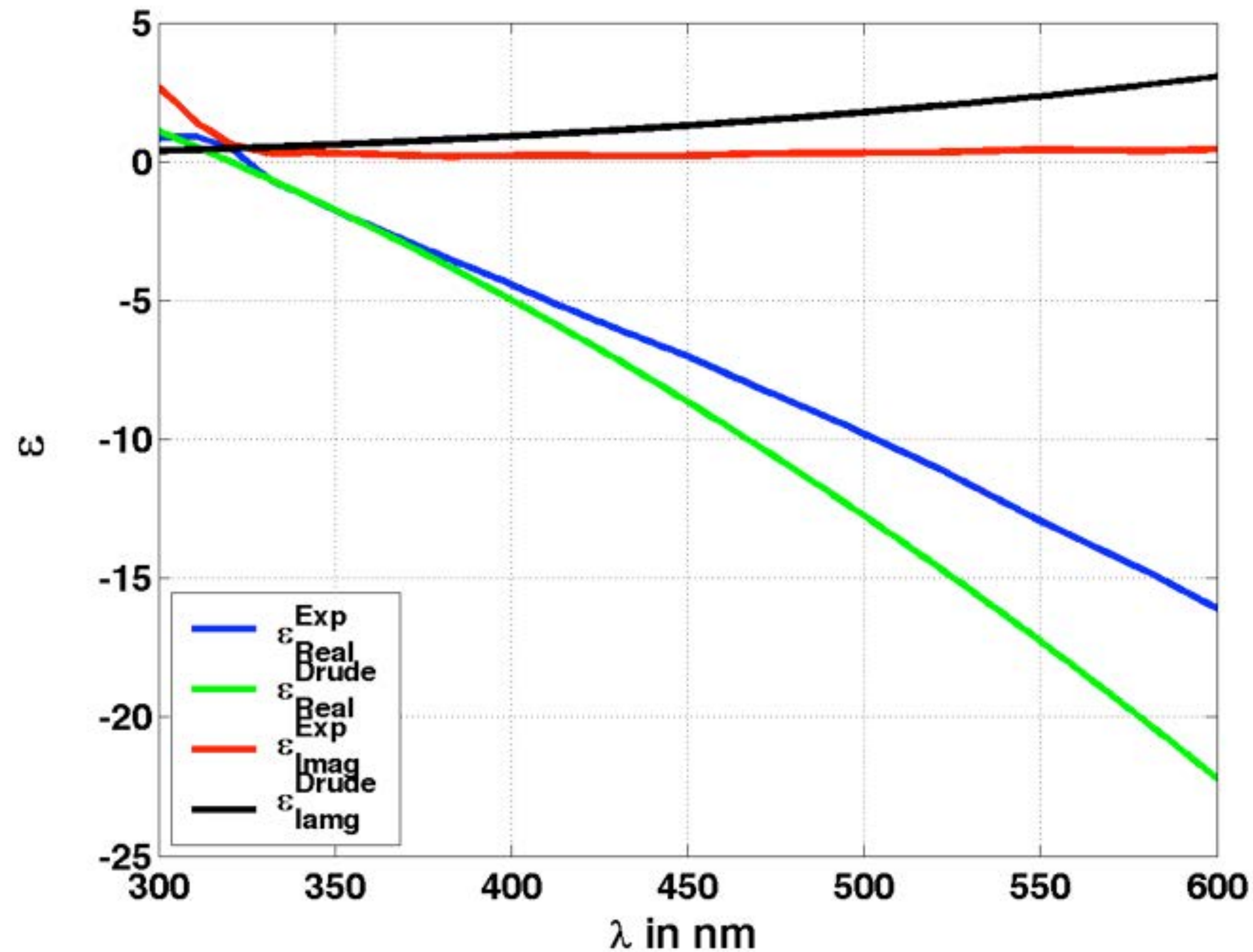
$$\nabla \times \mathbf{H} = \epsilon_{\mathrm{BG}} \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}$$

+ eqn. relating current and electric field (Drude model, mean drift velocity of electrons in a field)

$$\frac{\partial \mathbf{J}}{\partial t} + \gamma \mathbf{J} = \epsilon_0 \omega_{\mathrm{P}}^2 \mathbf{E}$$

ω_{P} ⟹ plasma frequency

$1/\gamma$ ⟹ relaxation time τ



$$\epsilon(\omega) = \epsilon_{\mathrm{BG}} - \frac{\omega_{\mathrm{P}}^2}{\omega^2 + i\gamma\omega}$$

FDTD for metals

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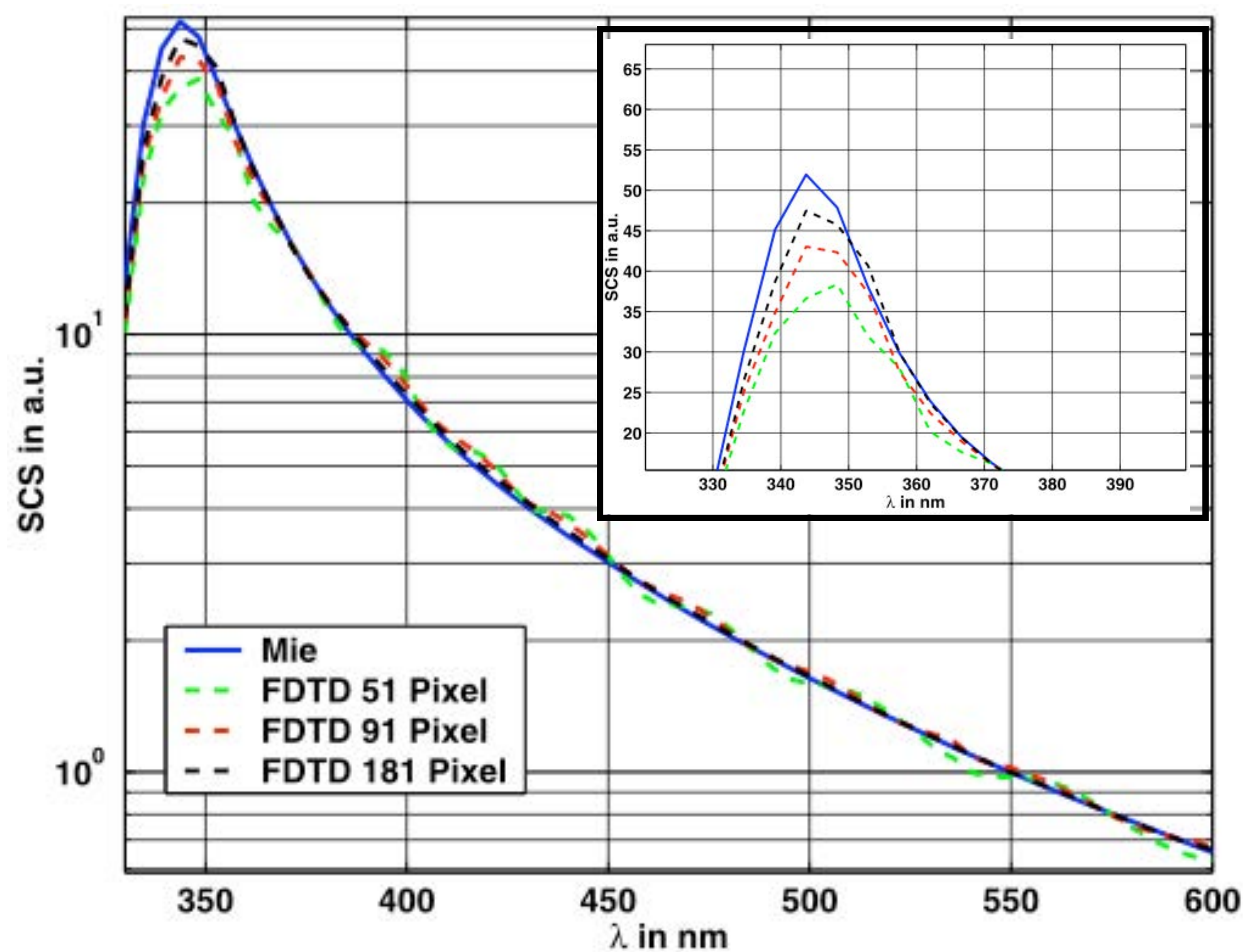


scattering cross section of a circular silver cylinder

(r=25nm, TM)

FDTD for Lorentz-materials

- assuming a 2D geometry (y-z-plane) with TM polarisation

$$\mathbf{E} = E_x \hat{x} \qquad \mathbf{P} = P_x \hat{x}$$

Lorentz dispersion (frequency domain)

(the same as Drude-model but resonance frequency is not at 0)

$$P_{x,\omega} = \frac{\epsilon_0 \omega_p^2 \chi_L}{\omega_0^2 - \omega^2 + j\omega\Gamma} E_{x,\omega}$$

Fourier-transformation

Lorentz dispersion (time domain)

$$\frac{\partial^2 P_x}{\partial t^2} + \Gamma \frac{\partial P_x}{\partial t} + \omega_0^2 P_x = \epsilon_0 \omega_p^2 \chi_L E_x$$

(R.W. Ziolkowski et al., JOSA A, Vol. 16, No. 4, 980)

FDTD for nonlinear/nondispersive materials

- going back to Maxwell's equations

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \cdot \mathbf{D} = \rho$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{j} \qquad \nabla \cdot \mathbf{B} = 0$$

⇨ linear: $\mathbf{D} = \epsilon\epsilon_0 \mathbf{E}$

instantaneous!

⇨ non-Linear: $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$

$$\mathbf{P} = \epsilon_0 \left[\hat{\chi}^{(1)} \mathbf{E} + \hat{\chi}^{(2)} \mathbf{E}^2 + \hat{\chi}^{(3)} \mathbf{E}^3 + \cdots \right]$$

FDTD for nonlinear/nondispersive materials

- example of an instantaneous Kerr $\hat{\chi}^{(3)}$ nonlinearity

$$D = \epsilon_0 \epsilon E \qquad \begin{aligned} \epsilon &= n^2 \\ &= (n_0 + n_2 |E|^2)^2 \\ &\simeq n_0^2 + 2 n_0 n_2 |E|^2 \end{aligned}$$

nonlinear refractive index depends on the square of the E-Field $(n_2 \ll n_0)$

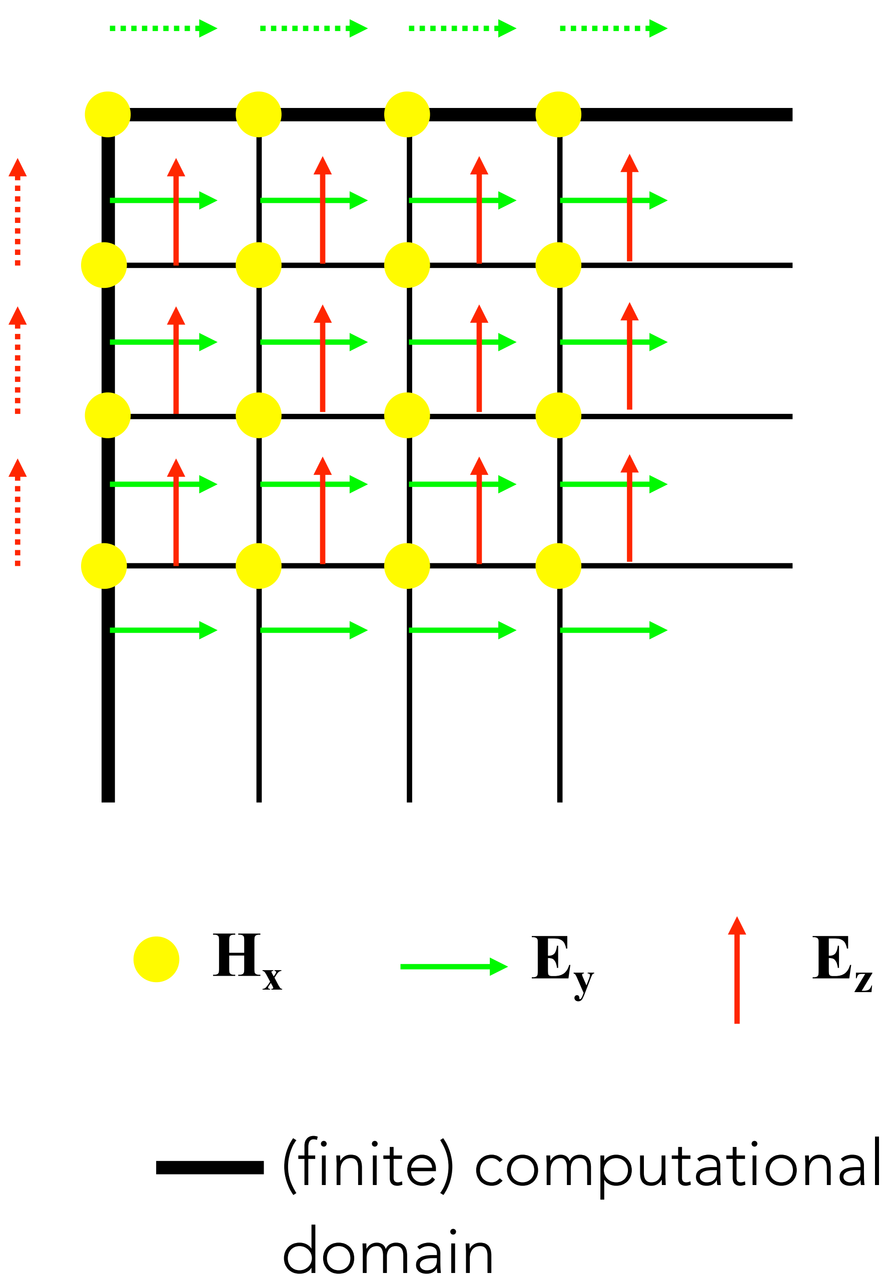
$$\boxed{E = \frac{D}{n_0^2 + 2 n_0 n_2 |E|^2}}$$

solution by a Newton iterative procedure (or direct)

$\Longrightarrow$ straight forward applicable to instantaneous $\hat{\chi}^{(2)}$ media

Boundary conditions

- problems appear if the fields at the boundary have to be evaluated



- for keeping the discretized mesh treatable on a computer, we have to limit its size

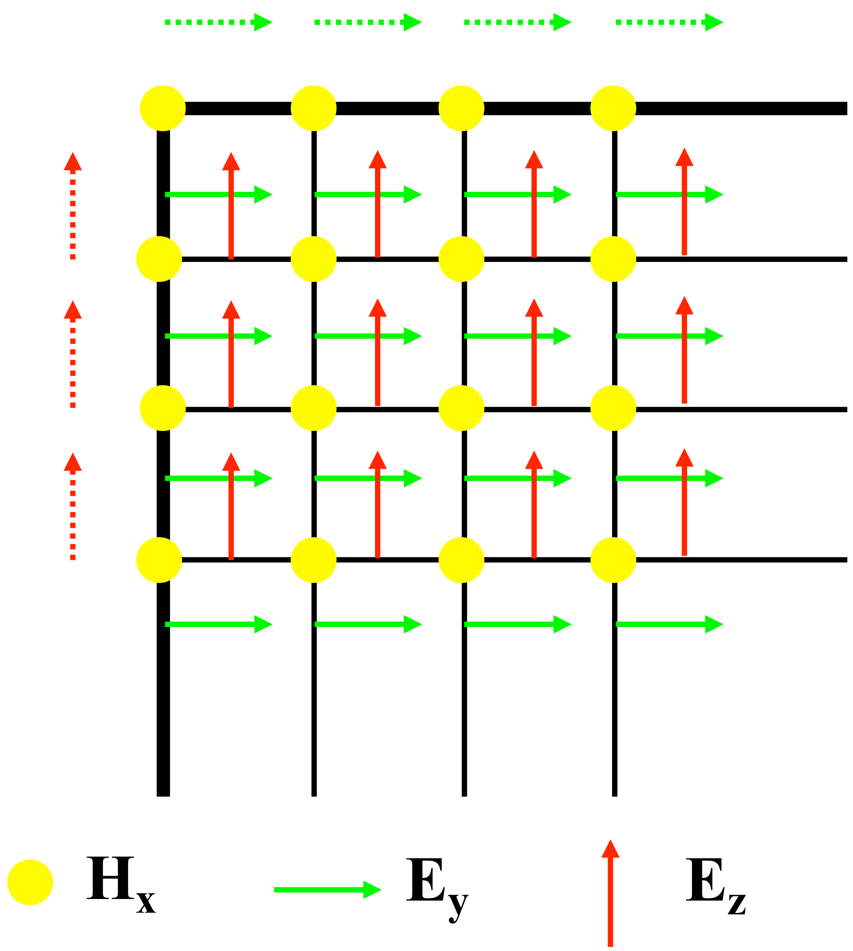
but

- for a proper determination of the field components that are positioned directly at the boundary of the computational domain, we need actually information about field components outside

⇨ choosing proper boundary conditions

Boundary conditions

- easiest boundary conditions: perfectly conducting material (E or H)



(physical grid)

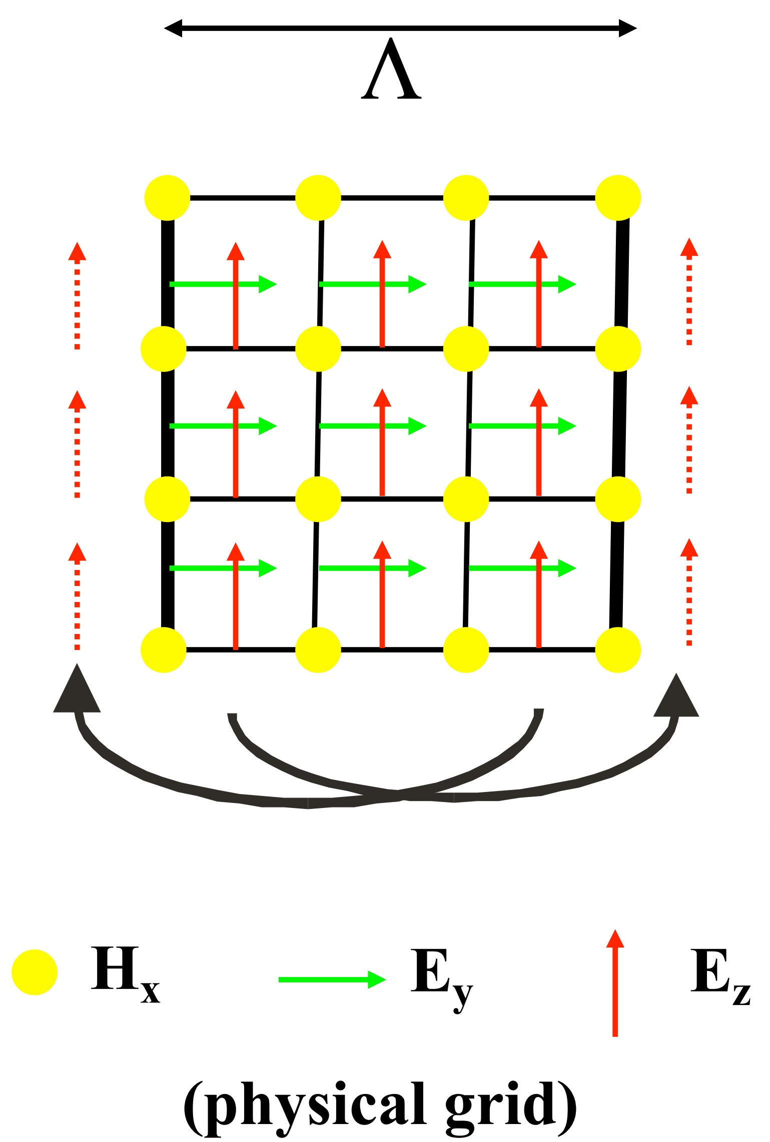
field cannot penetrate the structure

setting the field values outside the structure equal to zero

$$H_x^{n+\frac{1}{2}}(j+\frac{1}{2},k+\frac{1}{2}) = H_x^{n-\frac{1}{2}}(j+\frac{1}{2},k+\frac{1}{2}) + \frac{\Delta t}{\mu(j+\frac{1}{2},k+\frac{1}{2})\Delta z}[E_y^n(j,k+\frac{1}{2}) - \cancel{E_y^n(j,k-\frac{1}{2})}] - \frac{\Delta t}{\mu(j+\frac{1}{2},k+\frac{1}{2})\Delta y}[E_z^n(j+\frac{1}{2},k) - \cancel{E_z^n(j-\frac{1}{2},k)}]$$

Boundary conditions

- Floquet-Bloch boundaries for periodic objects (gratings, photonic crystals)



- Incident plane wave (arbitrary propagation direction)

$$E^{\mathrm{Inc}} \propto e^{ik_x x} e^{ik_y y} e^{ik_z z} e^{-i\omega t}$$

- Floquet-Bloch boundaries in the frequency domain (in x-direction)

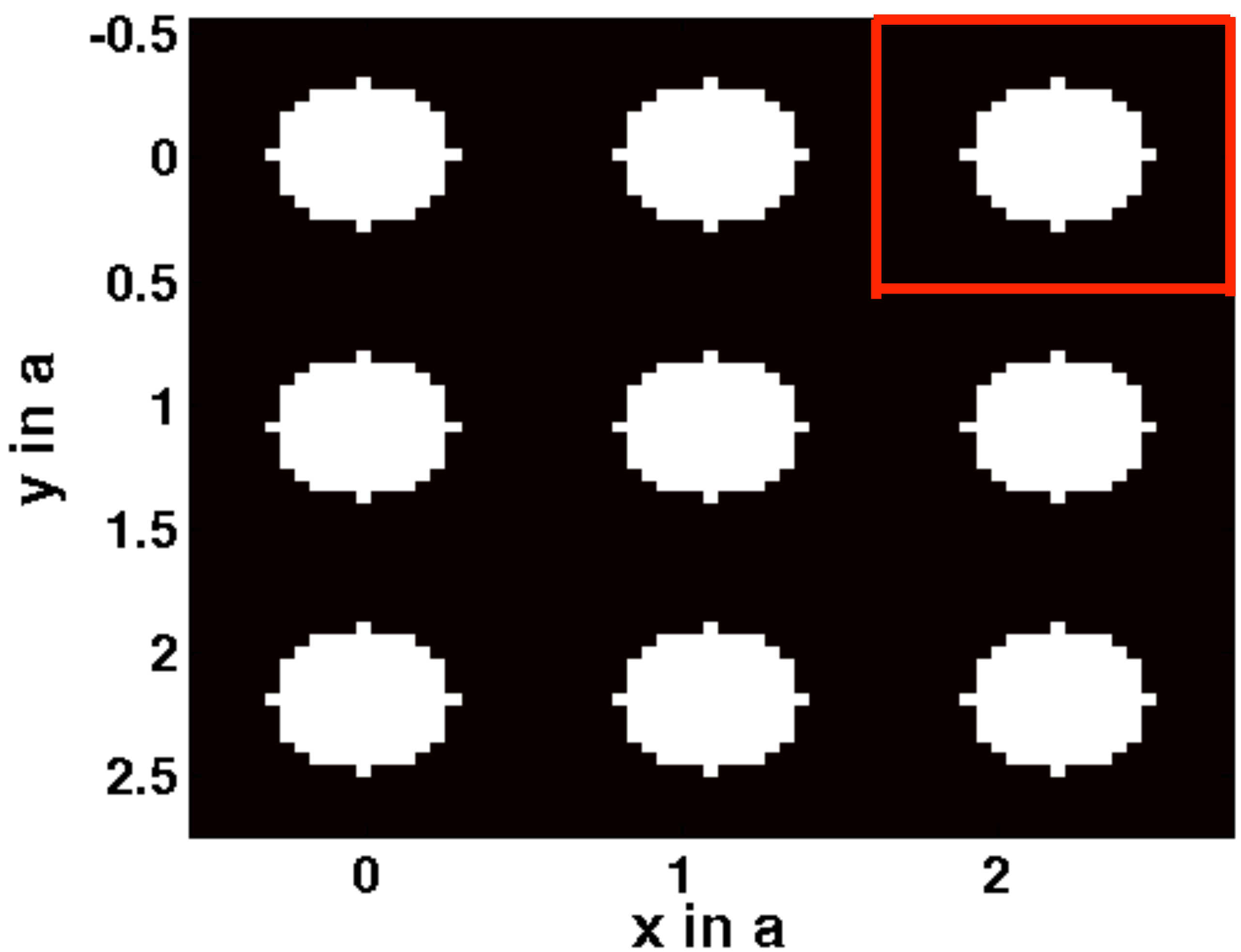
$$E\left(x+\Lambda_x, y, z, t\right) = E\left(x, y, z, t\right) e^{ik_x \Lambda_x}$$

- amplitude of the field displaced by one unit cell is identical, necessary since individual unit cells of a periodic structure is indistinguishable

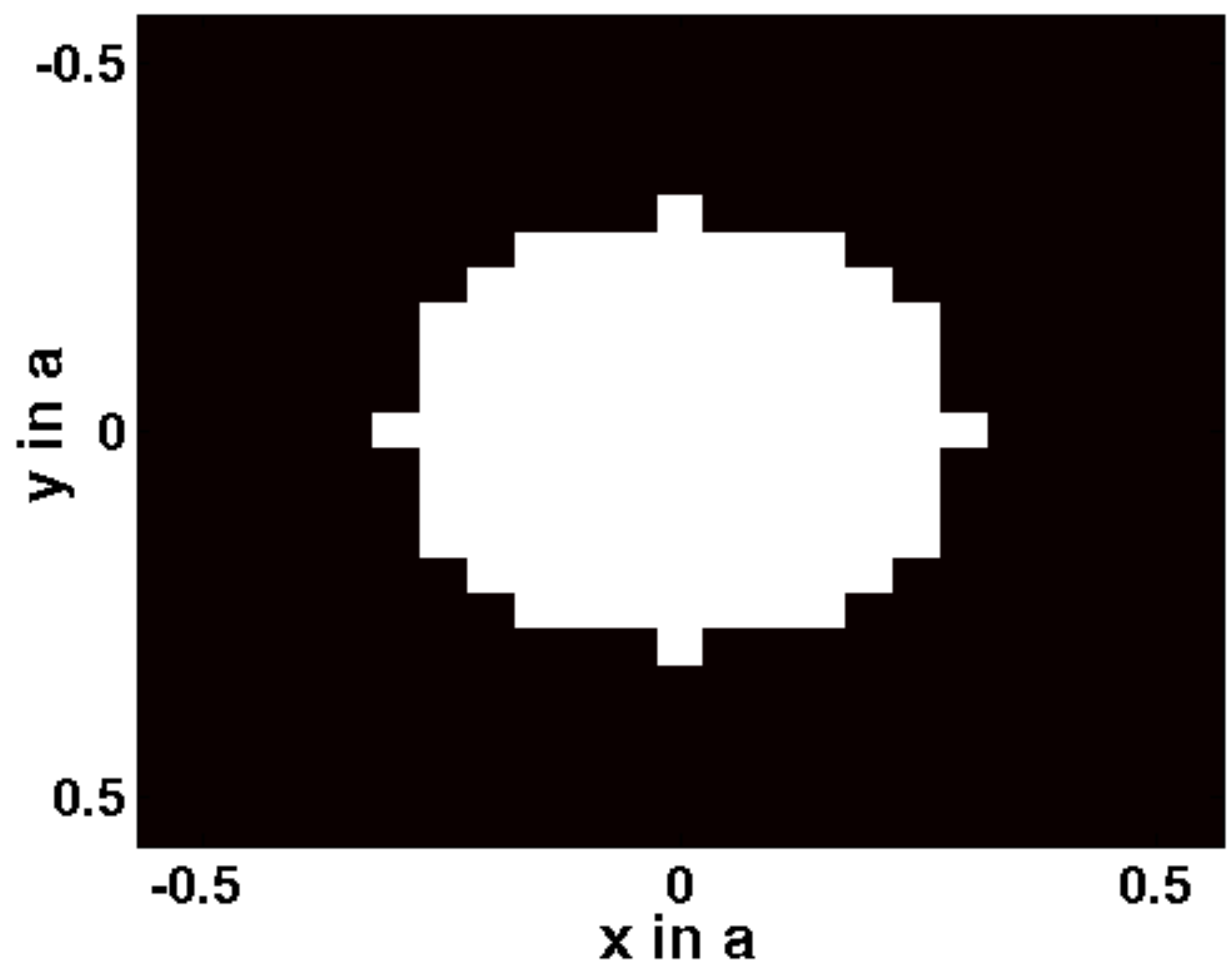
- only the phase changes by what is known as the Bloch phase

Boundary conditions

- Floquet-Bloch boundaries for calculating the band structure of a PC



geometry of a PC

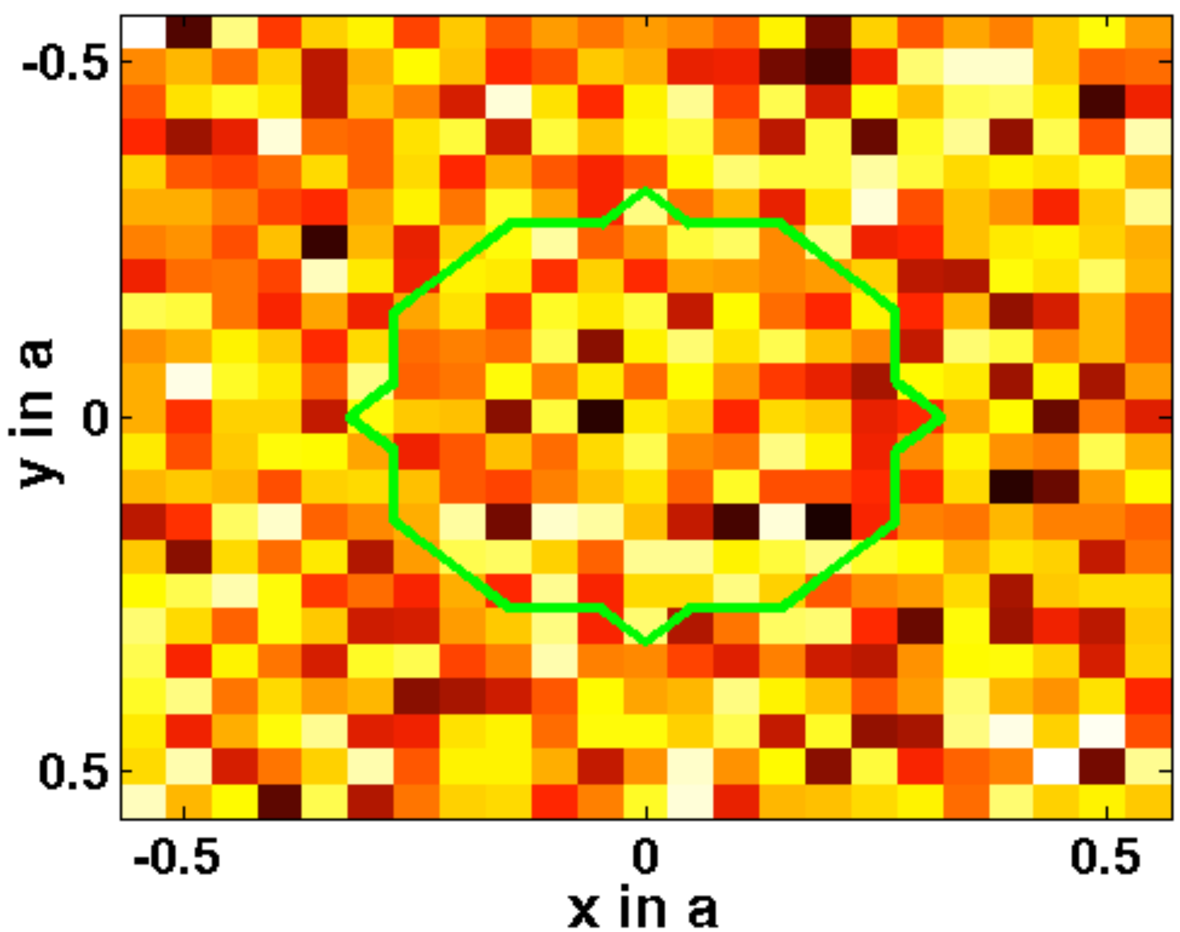


unit cell with cylindrical inclusion

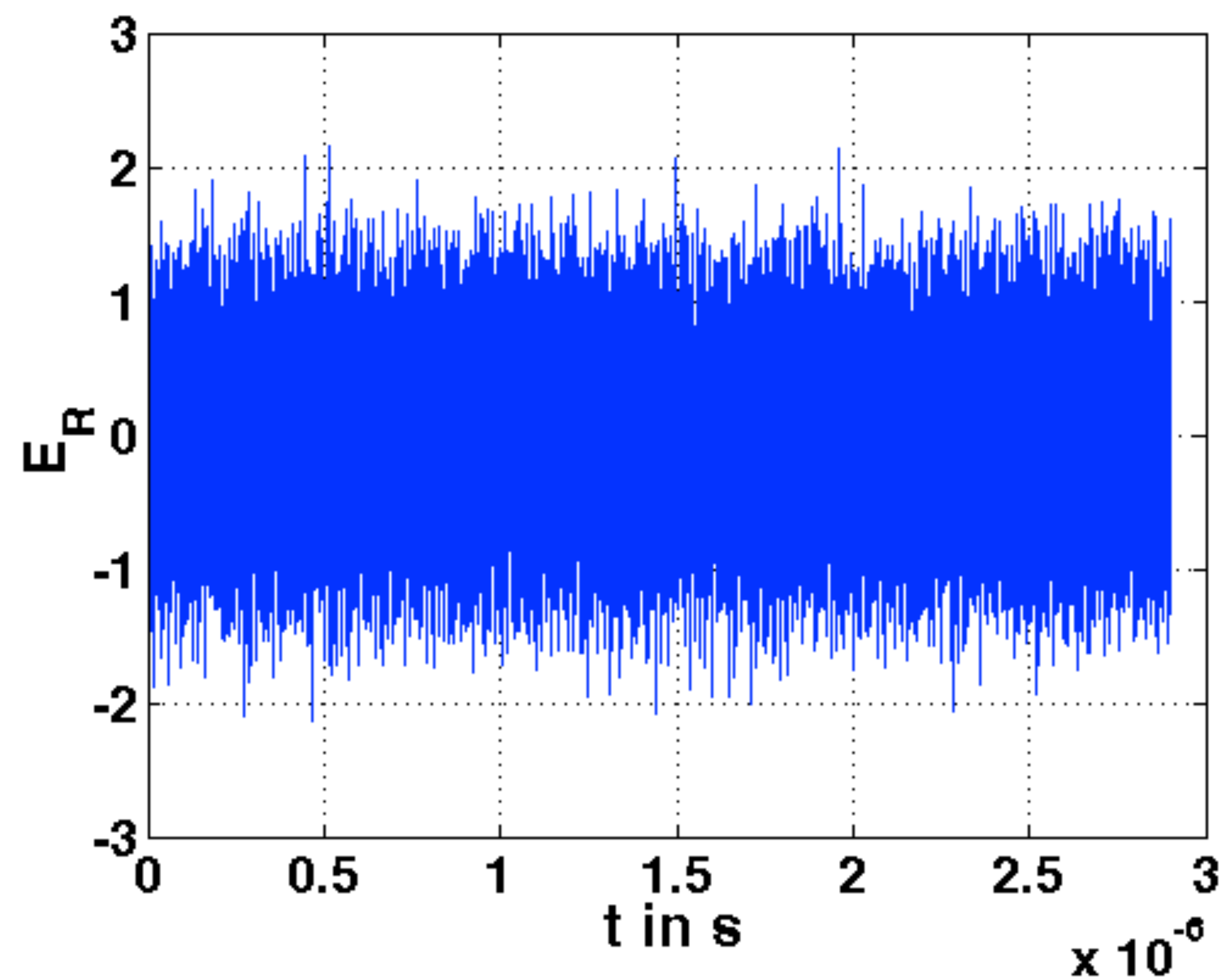
— periodic boundary with a particular k_x and k_y

Boundary conditions

- launching an arbitrary field distribution and recording the evolving pattern on some discrete points in the space



initial field distribution

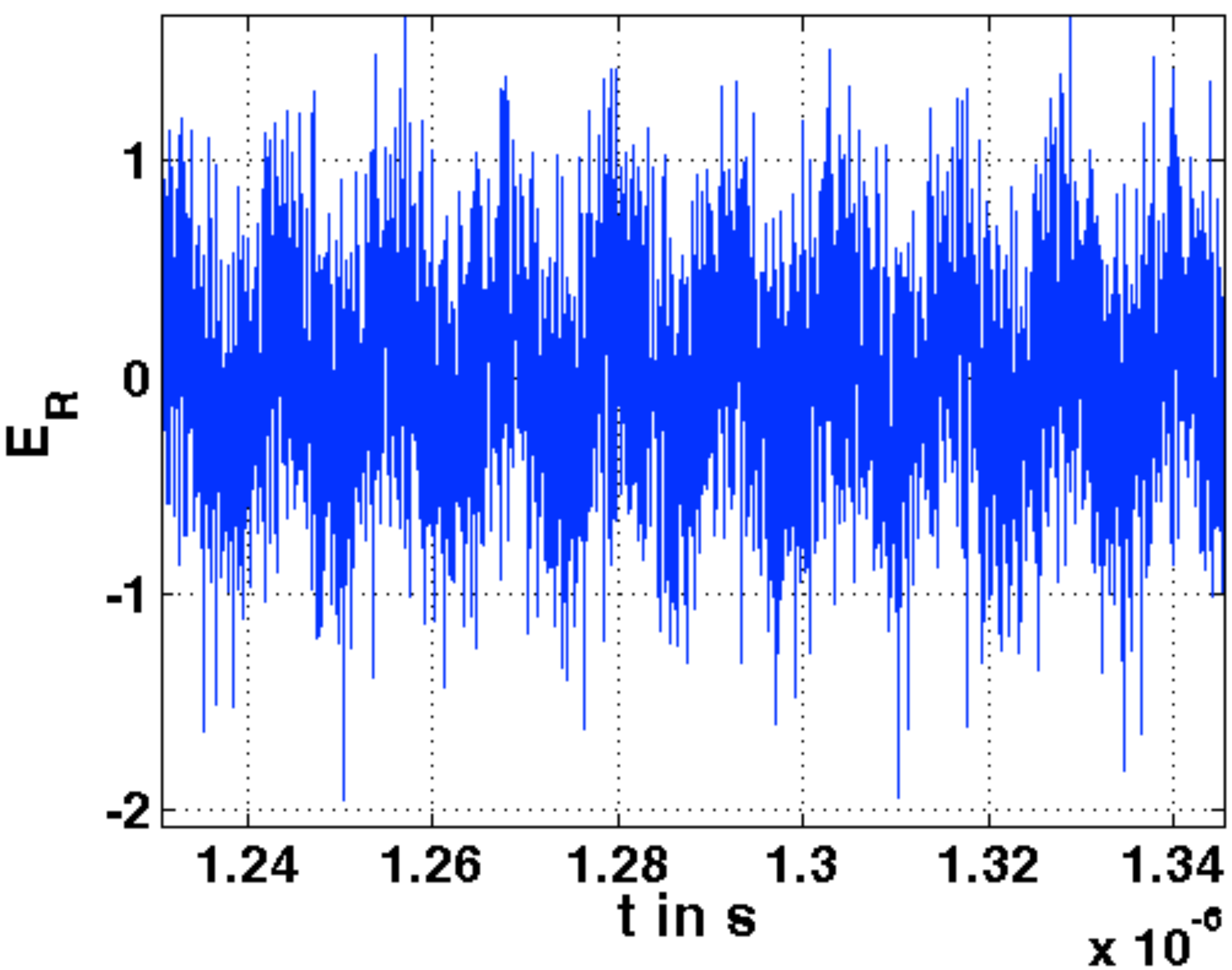


time evolution of the field

$$(\epsilon = 13, R = 0.3a)$$

Boundary conditions

- launching an arbitrary field distribution and recording the evolving pattern on some discrete points in the space



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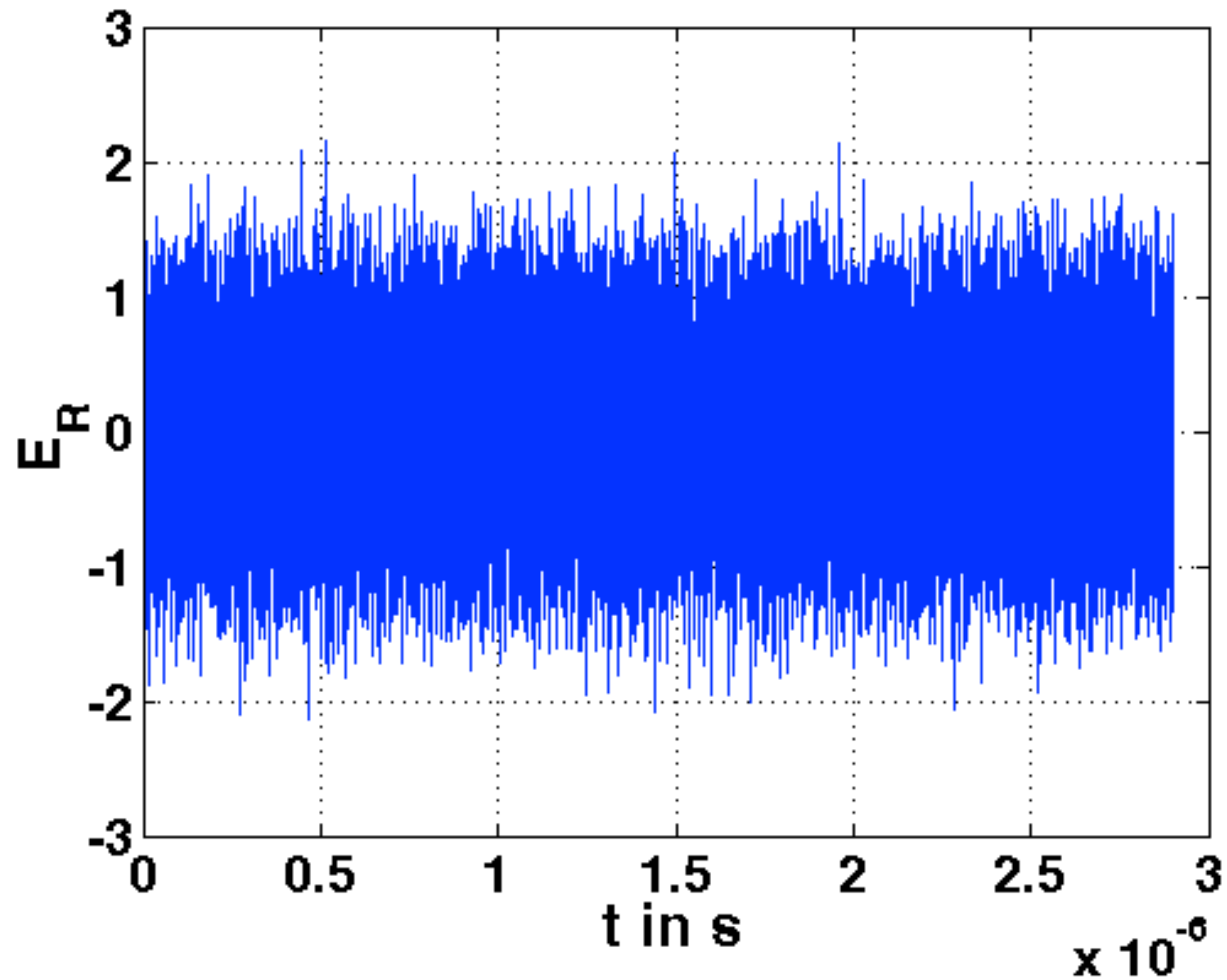
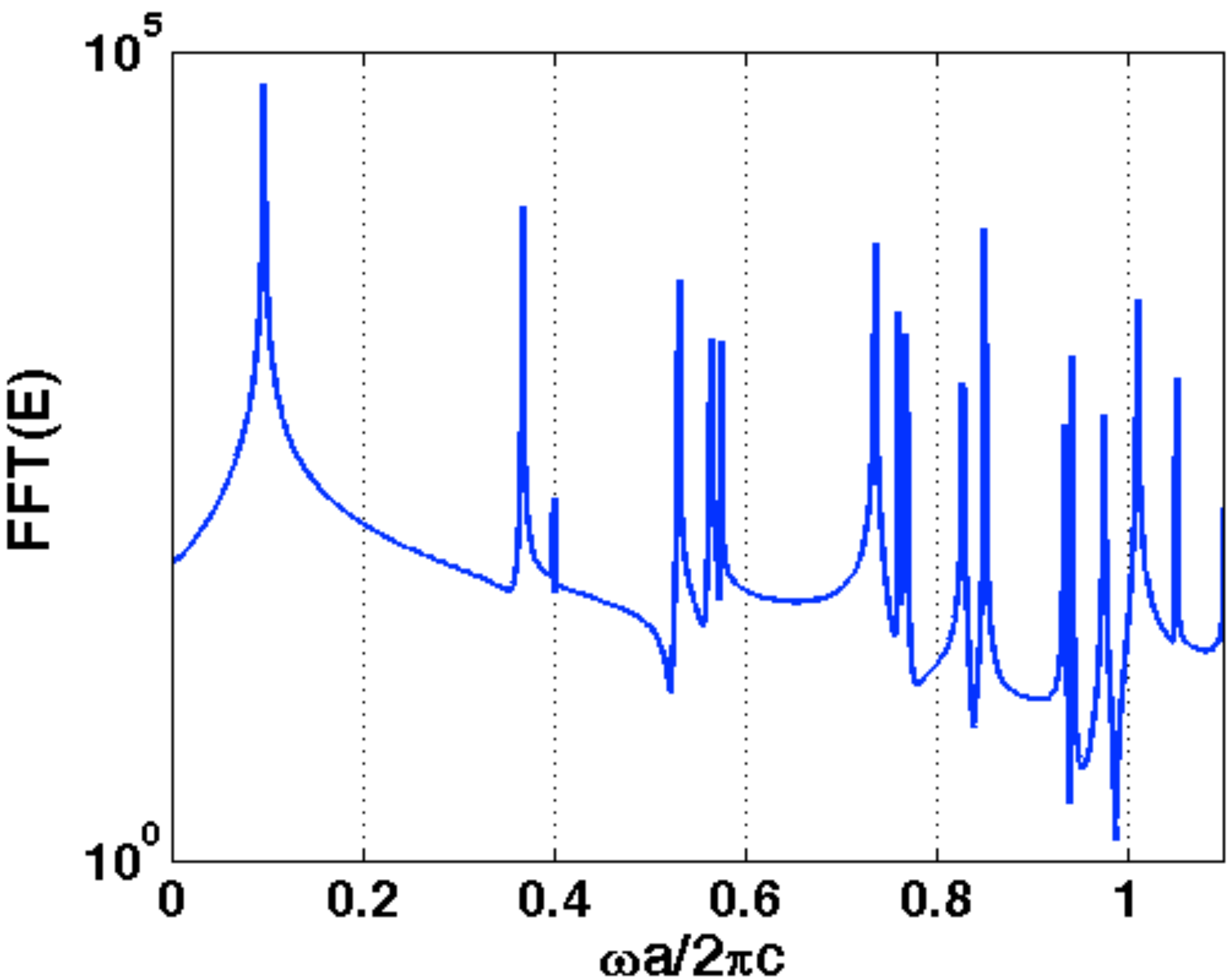


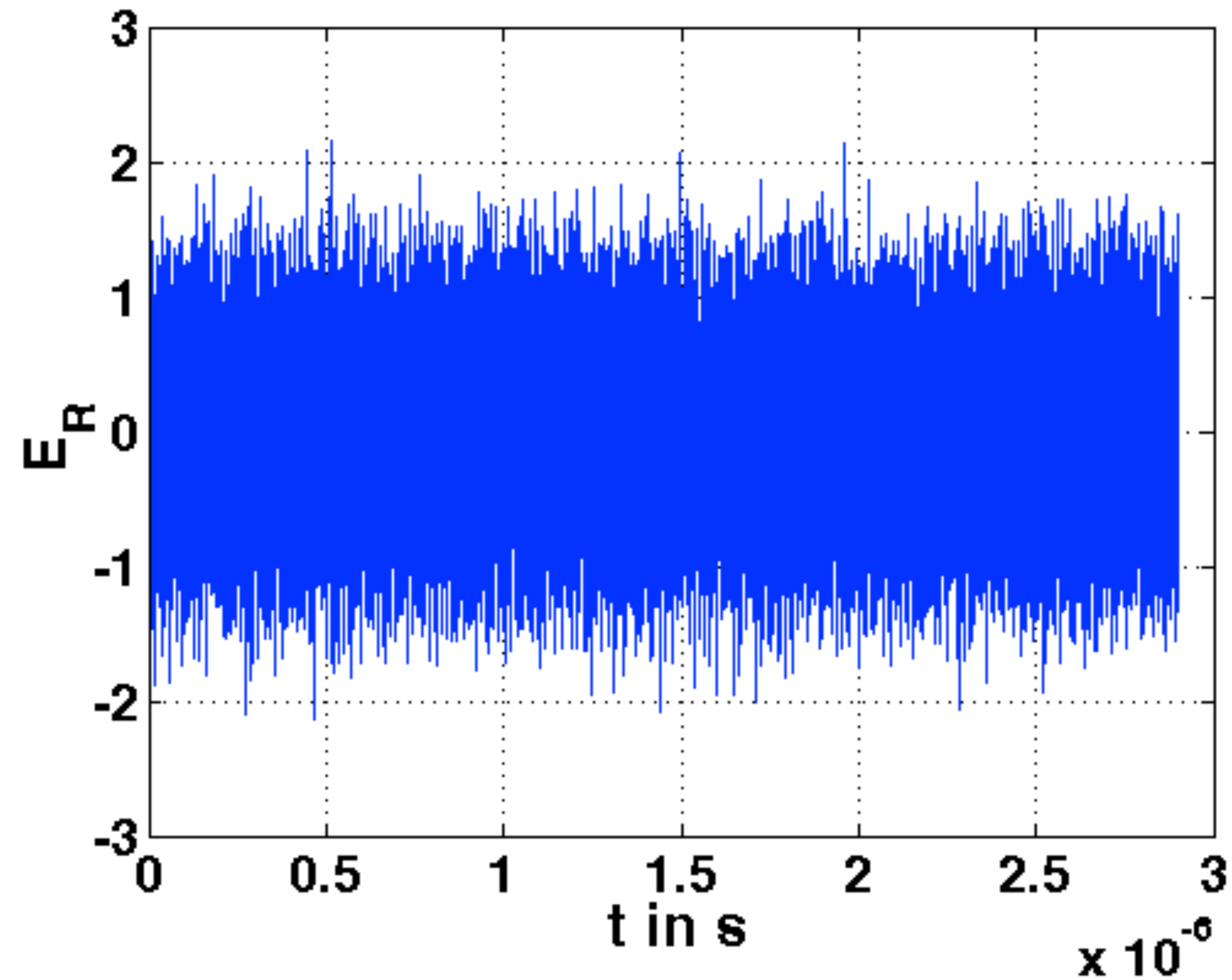
time evolution of the field

$$(\epsilon = 13, R = 0.3a)$$

Boundary conditions

- all the frequencies which do not satisfy the periodic boundaries are annihilated and only the modes that are allowed to propagate persist





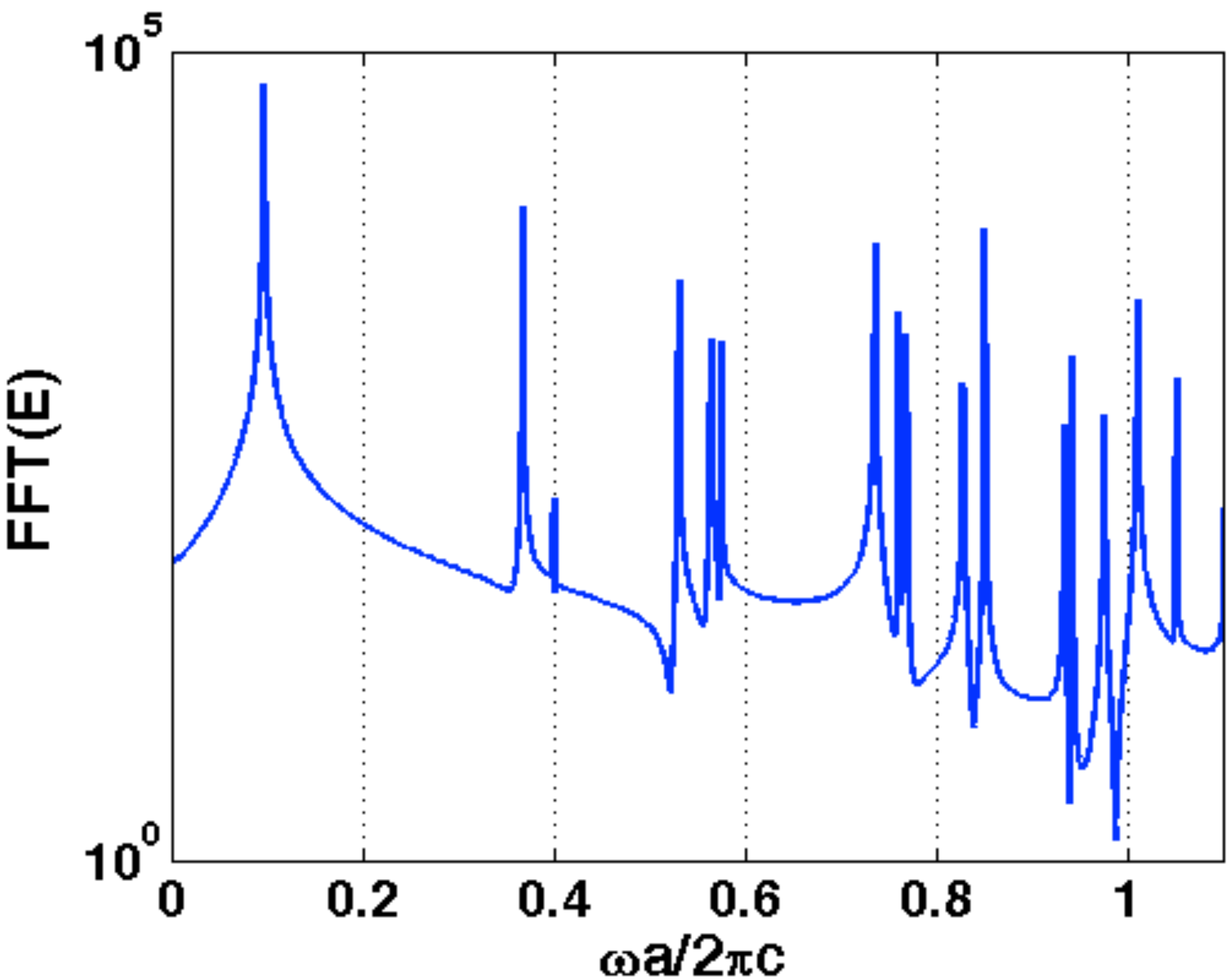
spectra obtained as a FFT

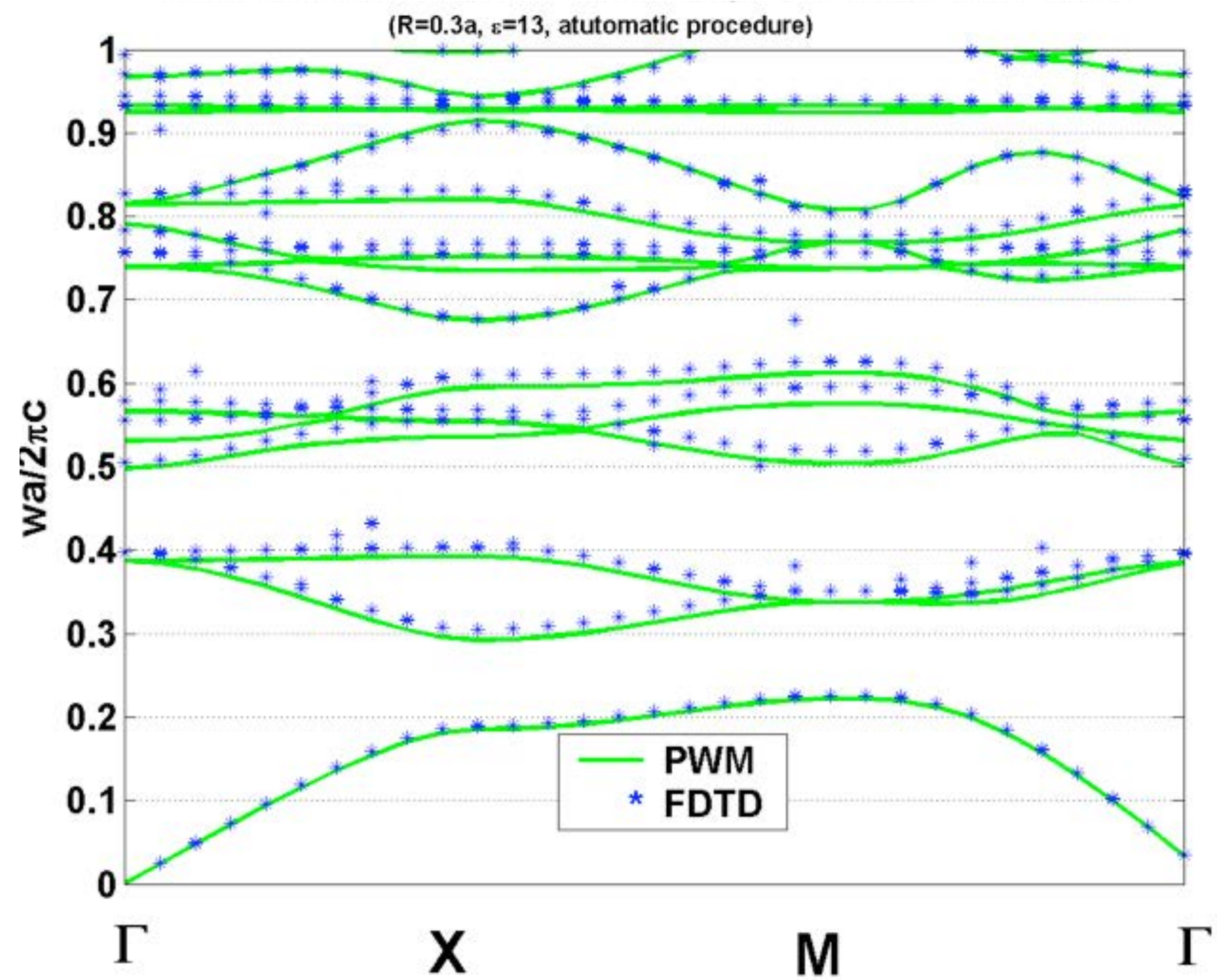
time evolution of the field

$$(\epsilon = 13, R = 0.3a)$$

Boundary conditions

- scanning the k-space and tracing the frequencies that persist as modes delivers the band structure via FDTD





spectra obtained as a FFT

band structure computation

$$(\epsilon = 13, R = 0.3a)$$

Boundary conditions

- neglecting the vectorial aspect: each field component obeys a scalar wave equation

$$\frac{\partial^2 f}{\partial x^2}+\frac{\partial^2 f}{\partial y^2}+\frac{\partial^2 f}{\partial z^2}-\frac{1}{c^2}\frac{\partial^2 f}{\partial t^2}=0 \qquad Lf=0$$

with

$$L=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}=\partial_x^2+\partial_y^2+\partial_z^2-c^{-2}\partial_t^2$$

$$\boxed{LU=L^{+}L^{-}U=0}$$

Boundary conditions

- for propagation in the +/- x-direction the operators are written as

$$L^{-} = \partial_x - c^{-1}\partial_t\sqrt{1-S^2}$$ ⟹ wave propagating in the –x-direction

$$L^{+} = \partial_x + c^{-1}\partial_t\sqrt{1-S^2}$$ ⟹ wave propagating in the +x-direction

$$S^2 = \left(\frac{\partial_y}{c^{-1}\partial_t}\right)^2 + \left(\frac{\partial_z}{c^{-1}\partial_t}\right)^2$$

$$\boxed{L^{-} f = 0}$$

Engquist-Madja exact ABC
(Mathematics of Computation, Vol. 31, 629, 1977)

- direct implementation of operator not possible, but the square-root can be expanded as a Taylor-series

Boundary conditions

$$(1-S^2)^{1/2} = 1 - \frac{1}{2}S^2 + O(S^4)$$

first order approximation

$$\cancel{S^2 = \left(\frac{\partial_y}{c^{-1}\partial_t}\right)^2 + \left(\frac{\partial_z}{c^{-1}\partial_t}\right)^2}$$

nearly plane wave propagating in x-direction

$$\boxed{L^- f = \partial_x f - c^{-1}\partial_t f = 0}$$

Boundary conditions

$$(1-S^2)^{1/2} = 1-\frac{1}{2}S^2 + O(S^4)$$

Second order approximation

$$(1-S^2)^{1/2} \approx 1-\frac{1}{2}S^2$$

$$S^2 = \left(\frac{\partial_y}{c^{-1}\partial_t}\right)^2 + \left(\frac{\partial_z}{c^{-1}\partial_t}\right)^2$$

$$L^- = \partial_x - \frac{\partial_t}{c} + \frac{1}{2}\frac{c}{\partial_t}\left(\partial_y^2 + \partial_z^2\right)$$

$$L^- f = \partial_{xt}^2 f - c^{-1}\partial_{tt}^2 f + 0.5c(\partial_{yy}^2 f + \partial_{zz}^2 f) = 0$$

Boundary conditions

- writing the differential operators as finite differences
  (G. Mur, IEEE Trans. Electromagnetic Compatibility, Vol. 32, 377, 1981)
- discretising the operator a half spatial step in front of the boundary
  (example of the boundary at x=0)

$$\partial^2_{xt} f \Big|^{n}_{1/2,j,k} = \frac{1}{2\Delta t}\left(\frac{f^{n+1}_{1,j,k} - f^{n+1}_{0,j,k}}{\Delta x} - \frac{f^{n-1}_{1,j,k} - f^{n-1}_{0,j,k}}{\Delta x} \right)$$

- averaging the second time derivatives at x=0 and x=Δx

$$\partial^2_t f = \frac{1}{2}\left[\frac{f^{n+1}_{0,j,k} - 2 f^{n}_{0,j,k} + f^{n-1}_{0,j,k}}{\Delta t^2} + \frac{f^{n+1}_{1,j,k} - 2 f^{n}_{1,j,k} + f^{n-1}_{1,j,k}}{\Delta t^2} \right]$$

- same holds for the second time derivatives in y and z direction

Boundary conditions

- inserting all those difference scheme leads to

$$
\begin{aligned}
f^{n+1}_{0,j,k} = -f^{n-1}_{0,j,k} &+ k_1(f^{n+1}_{1,j,k} + f^{n-1}_{0,j,k}) + k_2(f^{n}_{1,j,k} + f^{n}_{0,j,k}) + \\
&k_{3y}(f^{n}_{0,j-1,k} - 2f^{n}_{0,j,k} + f^{n}_{0,j+1,k} + f^{n}_{1,j-1,k} - 2f^{n}_{1,j,k} + f^{n}_{1,j+1,k}) + \\
&k_{3z}(f^{n}_{0,j,k-1} - 2f^{n}_{0,j,k} + f^{n}_{0,j,k+1} + f^{n}_{1,j,k-1} - 2f^{n}_{1,j,k} + f^{n}_{1,j,k+1})
\end{aligned}
$$

$$
k_1 = \frac{c\Delta t - \Delta x}{c\Delta t + \Delta x} \qquad k_2 = \frac{2\Delta x}{c\Delta t + \Delta x} \qquad k_{3y} = \frac{(c\Delta t)^2 \Delta x}{2\Delta y^2(x\Delta t + \Delta x)}
$$

- example for boundary x=0, similar equations for other boundaries
- fields have to be stored for 2 different time steps

Boundary conditions

- simplification by using only the first order Taylor approximation
(skipping the derivatives along the y and z directions)

$$f_{0,j,k}^{n+1} = -f_{0,j,k}^{n-1} + k_1(f_{1,j,k}^{n+1} + f_{0,j,k}^{n-1}) + k_2(f_{1,j,k}^{n} + f_{0,j,k}^{n})$$

- only the fields components that are evaluated at this (most outer) boundary have to be updated with this equation
(the tangential components of the E-field e.g. at the boundary x=0)

  - reflection coefficients are in the order of 10^{-2}

- easy to implement

Computational Photonics

Finite-Difference Time-Domain