Maxwellsche Gleichungen [makroskopisch]

$$\mathrm{rot}\big(\vec{E}(\vec{r},t)\big) + \frac{\partial}{\partial t}\vec{B}(\vec{r},t) = 0 \qquad \mathrm{rot}\big(\vec{H}(\vec{r},t)\big) - \frac{\partial}{\partial t}\vec{D}(\vec{r},t) = \vec{j}_{\mathrm{macr}}(\vec{r},t)$$

$$\mathrm{div}\big(\vec{D}(\vec{r},t)\big) = \rho_{\mathrm{ext}}(\vec{r},t) \qquad \mathrm{div}\big(\vec{B}(\vec{r},t)\big) = 0$$

And $\vec{D} = \varepsilon_0\vec{E} + \vec{P}$ and $\vec{B} = \mu_0\vec{H} + \vec{M}$. Nomenclatur: $\vec{E}$ - electric field, $\vec{D}$ - dielectric flux density, $\vec{P}$ - dielectric polarization, $\vec{H}$ - magnetic field, $\vec{B}$ - magnetic flux density, $\vec{M}$ - magnetic polarization, ρ_{ext} - external charge density, $\vec{j}_{\mathrm{macr}}$ - free current density, ε_0 - vacuum permittivity, μ_0 - vacuum permeability.

Fouriertransformation: $V(\vec{r},t) = \int_{-\infty}^{\infty}\tilde{V}(\vec{r},\omega)\,\mathrm{e}^{-\mathrm{i}\omega t}\,\mathrm{d}\omega$, $\tilde{V}(\vec{r},\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty}V(\vec{r},t)\,\mathrm{e}^{\mathrm{i}\omega t}\,\mathrm{d}t$. $[\Rightarrow\ \partial_t \hat{=} -\mathrm{i}\omega]$

For linear, homogenous, isotropic, nonmagnetic, ρ_{ext}- and $\vec{j}_{\mathrm{macr}}$-free media it follows in the frequency domain the **Helmholtz**-equation:

$$\Delta\tilde{\vec{E}} + \frac{\omega^2}{c^2}\varepsilon(\omega)\tilde{\vec{E}} = 0$$

$$\delta(x) = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{e}^{\mathrm{i}kx}\,\mathrm{d}k$$

At surfaces [without free charges and macroscopic currents] the following quantities are constant:

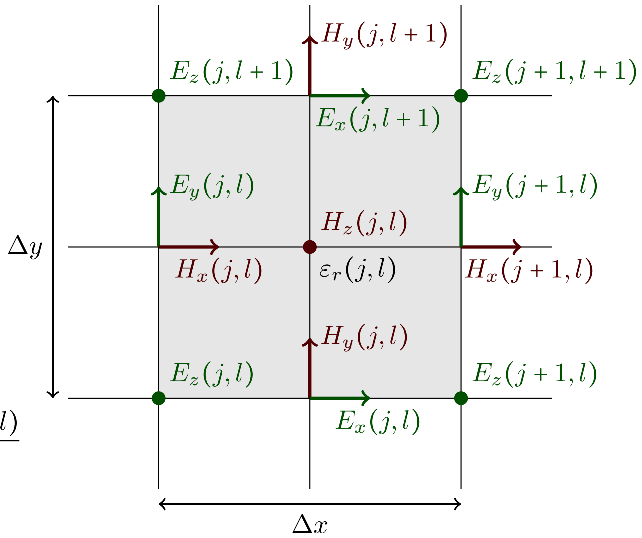
$$\vec{D}_\perp \ ,\ \vec{B}_\perp \ ,\ \vec{E}_\parallel \ \text{and}\ \vec{H}_\parallel \ .$$

For continous quantities as above a matrix-method can be used; however backreflexions are considered with this method and thus the field put into the algorithm might consist mainly out of backreflexions!

Numerical derivatives [Stencil notation]: $\partial_x = \frac{1}{2h}[-1\ 0\ 1]$, $\partial_x{}^2 = \frac{1}{h^2}[1\ -2\ 1]$.

In order to minimize the computational errors when calculating the $\vec{E}_{\mathrm{physical}}$ and $\vec{H}_{\mathrm{physical}}$ [the real physical fields in SI-units] one normalizes them with the free space impedance $Z_0 = \sqrt{\frac{\mu_0}{\epsilon_0}} \Rightarrow \vec{E}_{\mathrm{numerical}} = \vec{E}_{\mathrm{physical}}$ and $\vec{H}_{\mathrm{numerical}} = Z_0\vec{H}_{\mathrm{physical}}$. Then the values of $\vec{E}_{\mathrm{numerical}}$ and $\vec{H}_{\mathrm{numerical}}$ should be in the same order of magnitude.

Yee-grid-cell in 2D



2D:
Using the numerical fields $\tilde{\vec{E}}$ and $\tilde{\vec{H}}$, the ansatz $\tilde{\vec{E}}(\vec{r},t) = \vec{E}(\vec{r})\,\mathrm{e}^{\mathrm{i}[\beta z - \omega t]}$ and $\tilde{\vec{H}}(\vec{r},t) = \vec{H}(\vec{r})\,\mathrm{e}^{\mathrm{i}[\beta z - \omega t]}$, assuming a slowly varying amplitude $[\frac{\partial\vec{E}}{\partial z} \ll \mathrm{i}\beta\vec{E}$, $\frac{\partial\vec{H}}{\partial z} \ll \mathrm{i}\beta\vec{H}]$ and utilizing the Yee-grid it follows [$\varepsilon_r(j,l)$ is evaluated at the position of $H_z(j,l)$]:

$$ik_0H_x(j,l) = \frac{E_z(j,l+1) - E_z(j,l)}{\Delta y} - \mathrm{i}\beta E_y(j,l)$$

$$ik_0H_y(j,l) = \mathrm{i}\beta E_x(j,l) - \frac{E_z(j+1,l) - E_z(j,l)}{\Delta x}$$

$$ik_0H_z(j,l) = \frac{E_y(j+1,l) - E_y(j,l)}{\Delta x} - \frac{E_x(j,l+1) - E_x(j,l)}{\Delta y}$$

$$-ik_0\varepsilon_{rx}E_x(j,l) = \frac{H_z(j,l+1) - H_z(j,l)}{\Delta y} - \mathrm{i}\beta H_y(j,l)$$

$$-ik_0\varepsilon_{ry}E_y(j,l) = \mathrm{i}\beta H_x(j,l) - \frac{H_z(j+1,l) - H_z(j,l)}{\Delta x}$$

$$-ik_0\varepsilon_{rz}E_z(j,l) = \frac{H_y(j+1,l) - H_y(j,l)}{\Delta x} - \frac{H_x(j,l+1) - H_x(j,l)}{\Delta y}$$

with $\varepsilon_{rx}(j,l) = \frac{\varepsilon_r(j,l) + \varepsilon_r(j,l-1)}{2}$, $\varepsilon_{ry}(j,l) = \frac{\varepsilon_r(j,l) + \varepsilon_r(j-1,l)}{2}$ and $\varepsilon_{rz}(j,l) = \frac{\varepsilon_r(j,l) + \varepsilon_r(j-1,l-1) + \varepsilon_r(j-1,l) + \varepsilon_r(j,l-1)}{4}$.

By formulating this problem with matrices, plugging them into each other [i.e. numerically calculating rot(rot())] and additionally using the div()-equations, the eigenvalues β can be calculated.

General partial differential equations: $p\frac{\partial^2 f}{\partial x^2}+q\frac{\partial^2 f}{\partial x\partial y}+r\frac{\partial^2 f}{\partial y^2}+s\frac{\partial f}{\partial x}+t\frac{\partial f}{\partial y}+uf+v=0$, $\begin{cases} q^2 < 4pr & \text{, ellipcitc PDE} \\ q^2 = 4pr & \text{, parabolic PDE} \\ q^2 > 4pr & \text{, hyperbolic PDE} \end{cases}$.

elliptic → boundary value problem, hyperbolic and parabolic → initial value problem.

Beam Propagation Method [BPM, fully vectorial]:

When assuming a charge and current free, non-magnetic, linear, isotropic medium with a slowly varying index profile ε_r in $\vec{e}_z$ direction [$\left|\frac{\partial_z \varepsilon_r}{\varepsilon_r}\right| \ll \left|\frac{\partial_z E_z}{E_z}\right|$], a paraxial beam with propagation direction $\vec{e}_z$ of the form $\vec{\tilde{E}}(\vec{r},t) = \vec{E}\,\mathrm{e}^{\mathrm{i}[\omega t - k_0 n z]}$ or $\vec{E}(\vec{r},\omega) = \vec{e}_t\,\mathrm{e}^{-\mathrm{i}nk_0 z} + E_z\vec{e}_z$ [with $\vec{e}_t$ being transversal in the xy-plane] and a slowly varying amplitude [$\left|\partial_z^2\vec{e}_t\right| \ll \left|-2\,\mathrm{i}\,nk_0\partial_z\vec{e}_t\right|$] it follows

$$2\,\mathrm{i}\,k_0 n\partial_z\begin{pmatrix}e_x\\e_y\end{pmatrix} = \begin{bmatrix}P_{xx} & P_{xy}\\P_{yx} & P_{yy}\end{bmatrix}\begin{pmatrix}e_x\\e_y\end{pmatrix}$$

with $P_{xx} = \partial_x^2+\partial_y^2+k_0^2[\varepsilon_r - n^2] + \partial_x\left[\frac{1}{\varepsilon_r}[\partial_x\varepsilon_r]\right]$, $P_{xy} = \partial_x\left[\frac{1}{\varepsilon_r}[\partial_y\varepsilon_r]\right]$,

$P_{yx} = \partial_y\left[\frac{1}{\varepsilon_r}[\partial_x\varepsilon_r]\right]$ and $P_{yy} = \partial_x^2+\partial_y^2+k_0^2[\varepsilon_r - n^2] + \partial_y\left[\frac{1}{\varepsilon_r}[\partial_y\varepsilon_r]\right]$.

Semi-vectorial BPM:
If application is mainly linearly polarized then one component can be neglected [TE → $e_y = 0$, TM → $e_x = 0$]; it then however neglects coupling effects between the polarization directions.

Scalar BPM:
For a very low index contrast in a linearly polarized operating setup $\partial_x\varepsilon_r$ and $\partial_y\varepsilon_r$ are negligible small ⇒ $\partial_x\varepsilon_r \approx \partial_y\varepsilon_r \approx 0$.

Possible approximation: Alternating Direction Implicit [ADI] - reduce problem to lower dimensions [keep one component [x/y] fixed, propagate by Δz; then keep the other component fixed [y/x] and propagate by Δz; ... Much faster.

Boundary conditions:

- Fields = 0 at boundaries; corresponds to perfect reflection on the walls.
- Absorbing Boundary Conditions [ABC] - strongly rising imaginary value of the refractive index outside the examined region.
- Transparent Boundary Conditions [TBC] - artificially excite boundary corresponding to the outgoing field components.
- Perfectly Matched Layers [PML] - absorb all outgoing fields via a stack of perfectly matched layers [⇔ open setup].

Finite Difference Time Domain Method [FDTD]:

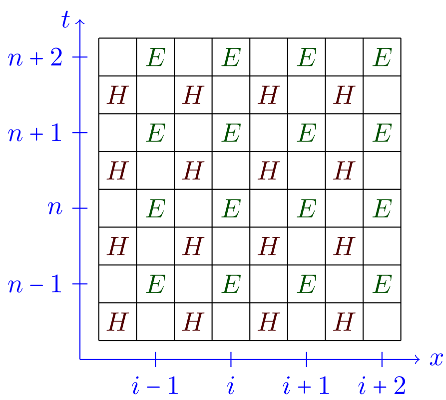
[typically: $\Delta t \sim 10^{-18}$ s, $\Delta x \sim 10^{-9}$ m]

Memory and time excessive computations. In exchange implementation of the computation scheme is rather simple; the setup however is rather cumbersome to implement [stability, boundary conditions, sources, ...].

1D: for a linear, isotropic, dispersionless and non-magnetic dielectric medium without macroscopic currents or free charges it follows from the rot()-Maxwell-equations using a symmetric discretization [Stencil $\partial_x \to \frac{1}{2\Delta x}[\ 1\quad 0\quad -1\ ]$ in both time- and space-domain; notation $\cdot(i\Delta x, n\Delta t) \to \cdot_i^n$]:

$$E_i^{n+1} = E_i^n + \frac{1}{\varepsilon_0\varepsilon_{ri}}\frac{\Delta t}{\Delta x}\left[H_{i+\frac{1}{2}}^{n+\frac{1}{2}} - H_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right] \quad ,$$

$$H_{i+\frac{1}{2}}^{n+\frac{1}{2}} = H_{i+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{1}{\mu_0}\frac{\Delta t}{\Delta x}\left[E_{i+1}^n - E_{i-1}^n\right] \quad .$$



Fields are automatically divergence-free if the polarisation of the fields is chosen orthogonal to the investigated space-coordinate.

3D: with the same assumptions as for the 1D case the equations below follow.

For perfectly conducting boundaries the boundary conditions are $\vec{E}_\parallel = \vec{0}$ and $\vec{H}_\perp = \vec{0}$ and therefore the dimensions are:

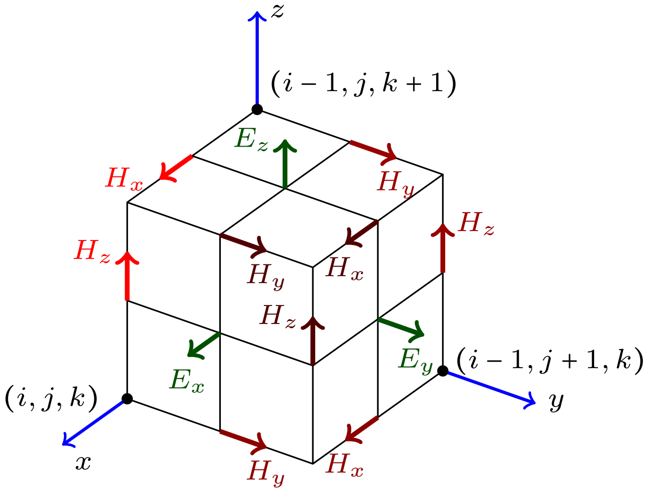
$$\begin{aligned} E_x^{n+\frac{1}{2}} &\to N_x, N_y+1, N_z+1 \quad , \quad H_x^n \to N_x+1, N_y, N_z \\ E_y^{n+\frac{1}{2}} &\to N_x+1, N_y, N_z+1 \quad , \quad H_y^n \to N_x, N_y+1, N_z \\ E_z^{n+\frac{1}{2}} &\to N_x+1, N_y+1, N_z \quad , \quad H_z^n \to N_x, N_y, N_z+1 \end{aligned}$$

It is $\partial_t \operatorname{div}(\vec{D}) = 0$ and $\partial_t \operatorname{div}(\vec{B}) = 0$ with this grid and thus the initial divergence-free nature of the fields conserved.

Computation scheme is called „leapfrog“.

Courant-Friedrichs-Lewy condition:

$$\Delta t \le \frac{1}{c}\left[\frac{1}{[\Delta x]^2} + \frac{1}{[\Delta y]^2} + \frac{1}{[\Delta z]^2}\right]^{-\frac{1}{2}}$$



Yee-grid-cell in 3D

Sources can be implemented via macroscopic currents $\vec{j}_{\text{macr}}$.

$$E_x\big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}} = E_x\big|^{n-\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\varepsilon_0\,\varepsilon_r\big|_{i,j+\frac{1}{2},k+\frac{1}{2}}}\left[\frac{1}{\Delta y}\left[H_z\big|^n_{i,j+1,k+\frac{1}{2}} - H_z\big|^n_{i,j,k+\frac{1}{2}}\right] - \frac{1}{\Delta z}\left[H_y\big|^n_{i,j+\frac{1}{2},k+1} - H_y\big|^n_{i,j+\frac{1}{2},k}\right] - j_x\big|^n_{i,j+\frac{1}{2},k+\frac{1}{2}}\right]$$

$$E_y\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+1,k+\frac{1}{2}} = E_y\big|^{n-\frac{1}{2}}_{i-\frac{1}{2},j+1,k+\frac{1}{2}} + \frac{\Delta t}{\varepsilon_0\,\varepsilon_r\big|_{i+\frac{1}{2},j+1,k+\frac{1}{2}}}\left[\frac{1}{\Delta z}\left[H_x\big|^n_{i-\frac{1}{2},j+1,k+1} - H_x\big|^n_{i-\frac{1}{2},j+1,k}\right] - \frac{1}{\Delta x}\left[H_z\big|^n_{i,j+1,k+\frac{1}{2}} - H_z\big|^n_{i-1,j+1,k+\frac{1}{2}}\right] - j_y\big|^n_{i-\frac{1}{2},j+\frac{1}{2},k+1}\right]$$

$$E_z\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+\frac{1}{2},k+1} = E_z\big|^{n-\frac{1}{2}}_{i-\frac{1}{2},j+\frac{1}{2},k+1} + \frac{\Delta t}{\varepsilon_0\,\varepsilon_r\big|_{i-\frac{1}{2},j+\frac{1}{2},k+1}}\left[\frac{1}{\Delta x}\left[H_y\big|^n_{i,j+\frac{1}{2},k+1} - H_y\big|^n_{i-1,j+\frac{1}{2},k+1}\right] - \frac{1}{\Delta y}\left[H_x\big|^n_{i-\frac{1}{2},j+1,k+1} - H_x\big|^n_{i-\frac{1}{2},j,k+1}\right] - j_z\big|^n_{i-\frac{1}{2},j+\frac{1}{2},k+1}\right]$$

$$H_x\big|^{n+1}_{i-\frac{1}{2},j+1,k+1} = H_x\big|^n_{i-\frac{1}{2},j+1,k+1} + \frac{\Delta t}{\mu_0}\left[\frac{1}{\Delta z}\left[E_y\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+1,k+\frac{3}{2}} - E_y\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+1,k+\frac{1}{2}}\right] - \frac{1}{\Delta y}\left[E_z\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+\frac{3}{2},k+1} - E_z\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+\frac{1}{2},k+1}\right]\right]$$

$$H_y\big|^{n+1}_{i,j+\frac{1}{2},k+1} = H_y\big|^n_{i,j+\frac{1}{2},k+1} + \frac{\Delta t}{\mu_0}\left[\frac{1}{\Delta x}\left[E_z\big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},k+1} - E_z\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+\frac{1}{2},k+1}\right] - \frac{1}{\Delta z}\left[E_x\big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{3}{2}} - E_x\big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}}\right]\right]$$

$$H_z\big|^{n+1}_{i,j+1,k+\frac{1}{2}} = H_z\big|^n_{i,j+1,k+\frac{1}{2}} + \frac{\Delta t}{\mu_0}\left[\frac{1}{\Delta y}\left[E_x\big|^{n+\frac{1}{2}}_{i,j+\frac{3}{2},k+\frac{1}{2}} - E_x\big|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}}\right] - \frac{1}{\Delta x}\left[E_y\big|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - E_y\big|^{n+\frac{1}{2}}_{i-\frac{1}{2},j+1,k+\frac{1}{2}}\right]\right]$$

For dispersion $n(\omega)$ has to be taken into account. Therefore the problem has to be treated, inserting different single frequency waves and evaluating the response [needs linear medium]!

For non-dispersive media [in the investigated wavelength-range] one can also sent in a very short pulse [→ wide spectrum], record the time-evolution at different points and look at the timely Fourier transform of them → frequency response of the system calculateable.

For nonlinear [non-dispersive] media ODE at every discretization point has to be solved self-consistently.

Boundaries: perfect electric walls, perfect magnetic walls, transparent, periodic, …

[e.g. Floquet-Bloch periodic boundaries: $\Psi(x + m\Lambda_x, y + n\Lambda_y, \omega) = \Psi(x, y, \omega)\,\mathrm{e}^{\mathrm{i}[k_x m\Lambda_x + k_y n\Lambda_y]}$, $m, n \in \mathbb{Z}$
or perfectly matched layer: complex impedance matching at boundaries]

Fiber-waveguides:

Approximations: weak guidance [$\Delta n \ll 1$, $\nabla \ln(\varepsilon_r) \approx 0$], linearly polarized fields. Then it follows for the transversal profile of the electric field [$u = u_\perp \, \mathrm{e}^{\mathrm{i}[\beta z - \omega t]}$, u one electric field component, $k_0 = \frac{2\pi}{\lambda_0}$, λ_0 free space wavelength]

$$[\Delta_\perp + [k_0^2 \varepsilon_r - \beta^2]] u_\perp = 0 \,. \qquad (\alpha)$$

For guided modes $u_\perp$ and $u_\perp'$ have to be continous and bound [$u_\perp(r \to \infty) \to 0$, $u(r = 0) < \infty$]. This is an eigenvalue-problem with eigenvalue β and „eigenvector“ $u_\perp$.

For non-degenerate β [i.e. $\beta_a \neq \beta_b$ for $a \neq b$] and normalized fields [$\int_{\mathbb{R}^2} u_a^2 \,\mathrm{d}A = 1$] it follows $\int_{\mathbb{R}^2} u_a u_b \,\mathrm{d}A = \delta_{a,b}$.

Fiber parameter [V-number]: $V = k_0 a \sqrt{n_{\mathrm{co}}^2 - n_{\mathrm{cl}}^2}$, a core radius, n_{co} core refractive index, n_{cl} cladding refr. ind..

With $U = a\sqrt{k_0^2 n_{\mathrm{co}}^2 - \beta^2}$, $W = \sqrt{\beta^2 - k_0^2 n_{\mathrm{cl}}^2}$ $[V^2 = U^2 + W^2]$, $n^2(r) = n_{\mathrm{co}}^2 - [n_{\mathrm{co}}^2 - n_{\mathrm{cl}}^2]\, f(\frac{r}{a})$, $f(\frac{r}{a}) \begin{cases} \leq 1 & , r \leq a \\ = 1 & , r > a \end{cases}$, $u_\perp(r,\varphi) = u_r(r) u_\varphi(\varphi)$, $\rho = \frac{r}{a}$ and $Y_m(\rho) := u_r(r)$ it follows from (α):

$$u_\varphi(\varphi) = C \cos(m\varphi + \varphi_0) \quad , m \in \mathbb{N} \quad ; \quad \frac{\partial^2 Y_m}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial Y_m}{\partial \rho} + [U^2 + V^2 f(\rho) - \frac{m^2}{\rho^2}]\, Y_m = 0 \,.$$

[The latter is called Bessel DGL]

For $f(\rho) = \begin{cases} 0 & , \rho \leq 1 \\ 1 & , \rho > 1 \end{cases}$ analytic solutions are $Y_m = \begin{cases} A J_m(U\rho) & , \rho \leq 1 \\ B K_m(W\rho) & , \rho > 1 \end{cases}$ with the continuity condition $W\, J_m(U)\, K_m'(W) - U\, J_m'(U)\, K_m(W) = 0$. Using $J_m'(U) = \frac{m}{U} J_m(U) - J_{m+1}(U)$ and $K_m'(W) = \frac{m}{W} K_m(W) - K_{m+1}(W)$ this can be transformed in an more easily solveable equation: $\dfrac{J_m(U)}{U J_{m+1}(U)} = \dfrac{K_m(W)}{W K_{m+1}(W)}$. Solutions only exist for discrete U / W $\rightarrow$ LP_{mp}-modes.

For a more complex index distribution function $f(\rho)$ with a new notation $Y_m(\rho) = \rho^m X_m(\rho)$ the boundary conditions are as follows:

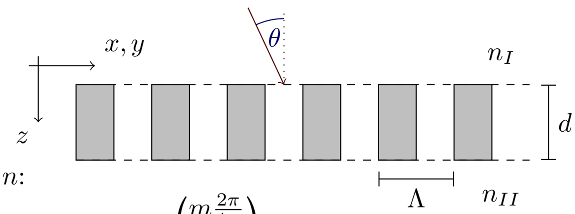
$$X_m(0) = c_m \,, X_m'(0) = 0 \text{ and } 0 = X_m'(1) - X_m(1)\left[W \frac{K_m'(W)}{K_m(W)} - m\right]$$

Using an equidistant discretization of ρ in the range $[0, 1]$ with stepsize $h = \frac{1}{N}$, the values at $\rho = 0$ can be numerically integrated to $\rho = 1$ employing an implicit mid-point Runge-Kutta method:

$$X_m(\rho_{j+1}) = X_m(\rho_j) + h \frac{\frac{h}{2}[V^2 f(\rho_j + \frac{h}{2}) - U^2] X_m(\rho_j) + \left.\frac{\mathrm{d}X_m(\rho)}{\mathrm{d}\rho}\right|_{\rho_j}}{1 + \frac{h}{2}\frac{2m+1}{\rho_j + \frac{h}{2}} - \frac{h^2}{4}[V^2 f(\rho_j + \frac{h}{2}) - U^2]} \quad ,$$

$$\left.\frac{\mathrm{d}X_m(\rho)}{\mathrm{d}\rho}\right|_{\rho_{j+1}} = \left.\frac{\mathrm{d}X_m(\rho)}{\mathrm{d}\rho}\right|_{\rho_j} + h \frac{[V^2 f(\rho_j + \frac{h}{2}) - U^2] X_m(\rho_j) + \left[\frac{h}{2}[V^2 f(\rho_j + \frac{h}{2}) - U^2] - \frac{2m+1}{\rho_j + \frac{h}{2}}\right] \left.\frac{\mathrm{d}X_m(\rho)}{\mathrm{d}\rho}\right|_{\rho_j}}{1 + \frac{h}{2}\frac{2m+1}{\rho_j + \frac{h}{2}} - \frac{h^2}{4}[V^2 f(\rho_j + \frac{h}{2}) - U^2]} \,.$$

By choosing different U and testing the integrated fields for the third boundary condition, it can be determined, whether the chosen U relate to physical fields or not. [shooting method]



Fourier Modal Method for transversally periodic systems:

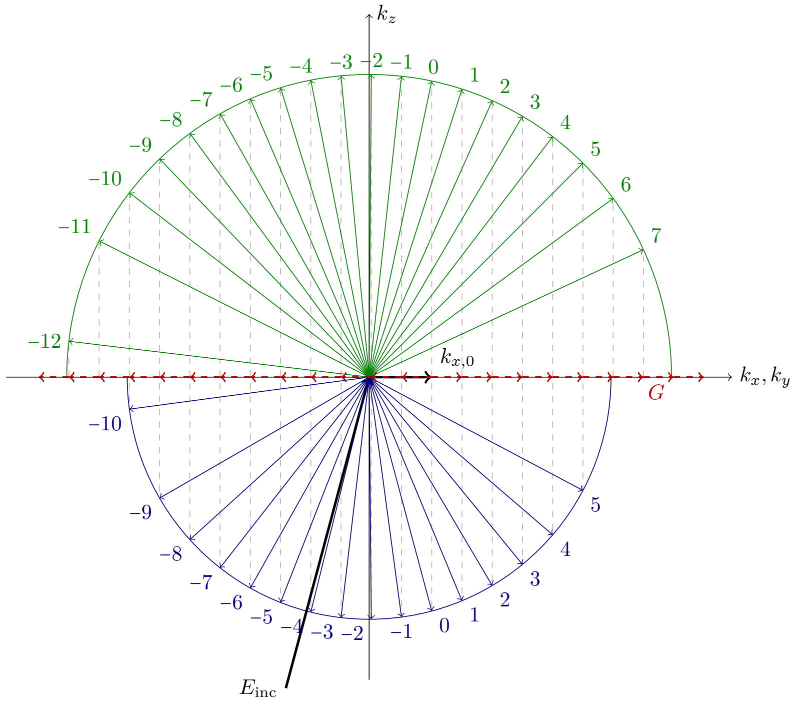
The grating [up to 2D] provides momenta for diffraction orders m, n:

$$k_{x,m} = k_{x,0} + G_{m0} \quad , \quad k_{y,n} = k_{y,0} + G_{0n} \quad , \quad \text{with} \quad G_{mn} = \begin{pmatrix} m\frac{2\pi}{\Lambda_x} \\ n\frac{2\pi}{\Lambda_y} \end{pmatrix} \,.$$

After scaling H_{phys} to $H = \frac{1}{Z_0} H_{\mathrm{phys}}$ and assuming monochromatic fields, Maxwell's curl equations read

$$\nabla \times E = \mathrm{i}\, k_0 H \quad , \quad \nabla \times H = -\,\mathrm{i}\, k_0 \varepsilon_r E \quad .$$

Via a spatially transversal Fourier decomposition $\alpha = \sum_{m,n} \alpha_{mn}\, \mathrm{e}^{\mathrm{i}\, G_{mn} r}$ for each quantity $\alpha \in \{E, H, \varepsilon_r, \frac{1}{\varepsilon_r}\}$ one gets



$$\partial_z E_{x,ij} = -\mathrm{i}\,\frac{k_{x,i}}{k_0}\sum_{c,d}\varepsilon^{-1}_{r;i-c,j-d}[k_{x,c}H_{y,cd} - k_{y,d}H_{x,cd}] + \mathrm{i}\,k_0 H_{y,ij} \quad ,$$

$$\partial_z E_{y,ij} = -\mathrm{i}\,\frac{k_{y,j}}{k_0}\sum_{c,d}\varepsilon^{-1}_{r;i-c,j-d}[k_{x,c}H_{y,cd} - k_{y,d}H_{x,cd}] - \mathrm{i}\,k_0 H_{x,ij} \quad ,$$

$$\partial_z H_{x,ij} = \mathrm{i}\,\frac{k_{x,i}}{k_0}[k_{x,i}E_{y,ij} - k_{y,j}E_{x,ij}] - \mathrm{i}\,k_0\sum_{c,d}\varepsilon_{r;i-c,j-d}E_{y,cd} \quad ,$$

$$\partial_z H_{y,ij} = \mathrm{i}\,\frac{k_{y,j}}{k_0}[k_{x,i}E_{y,ij} - k_{y,j}E_{x,ij}] + \mathrm{i}\,k_0\sum_{c,d}\varepsilon_{r;i-c,j-d}E_{x,cd} \quad .$$

And the z-components can be directly derived from the above quantities.

$$[H_{z,ij} = \frac{1}{k_0}[k_{x,i}E_{y,ij} - k_{y,j}E_{x,ij}] \quad , \quad E_{z,ij} = -\frac{1}{k_0}\sum_{c,d}\varepsilon^{-1}_{r;i-c,j-d}[k_{x,c}H_{y,cd} - k_{y,d}H_{x,cd}]]$$

Now one can assume a z-dependence of each guided mode a like $\mathrm{e}^{\mathrm{i}\,\beta_a z}$ and transform the above problem into matrix notation. One the gets

$$\partial_z\vec{E} = \hat{T}_1\vec{H} \quad , \quad \partial_z\vec{H} = \hat{T}_2\vec{E} \quad , \text{with } \vec{\alpha} = \begin{pmatrix}\vdots\\ \alpha_{x,ij}\\ \alpha_{y,ij}\\ \vdots\end{pmatrix} \quad , \alpha \in \{E, H\} \text{ and}$$

$$T_1^{ij,mn} = \frac{\mathrm{i}}{k_0}\begin{pmatrix} k_{x,i}\varepsilon^{-1}_{r;i-m,j-n}k_{y,n} & -k_{x,i}\varepsilon^{-1}_{r;i-m,j-n}k_{x,m} + k_0^2\delta_{ij,mn} \\ k_{y,j}\varepsilon^{-1}_{r;i-m,j-n}k_{y,n} - k_0^2\delta_{ij,mn} & -k_{y,n}\varepsilon^{-1}_{r;i-m,j-n}k_{x,m}\end{pmatrix} \quad \text{and}$$

$$T_2^{ij,mn} = \frac{\mathrm{i}}{k_0}\begin{pmatrix} -k_{x,i}k_{y,j}\delta_{ij,mn} & k_{x,i}^2\delta_{ij,mn} - k_0^2\varepsilon_{r;i-m,j-n} \\ -k_{y,j}^2\delta_{ij,mn} + k_0^2\varepsilon_{r;i-m,j-n} & k_{y,j}k_{x,i}\delta_{ij,mn}\end{pmatrix} \quad .$$

By compining the two equations one gets an eigenvalue problem: $[\vec{H} = \hat{T}_1^{-1}\partial_z\vec{E}]$

$$-\beta^2\vec{E} = \hat{T}_1\hat{T}_2\vec{E} \quad .$$

This can be numerically solved and thus yields the modes in the grating layer, expressed in the Fourier components. By considering additionally the boundary-conditions of the fields at the boundaries of the grating-layer [yields linear equation system for the Fourier components], the reflection and transmission of such a system can be derived. For the efficiencies it should be noted, that the square of the absolute amplitude has to be scaled according to the medium, in order to derive the correct efficiencies:

$$\eta_{\text{reflection},m} = |E_{\text{reflected},m}|^2\,\mathrm{Re}\left(\frac{k_{z,Im}}{k_{z,I0}}\right) \quad , \quad \eta_{\text{transmission},m} = |E_{\text{transmitted},m}|^2\,\mathrm{Re}\left(\frac{k_{z,IIm}}{\frac{n_{II}}{n_I}k_{z,I0}}\right) \quad .$$

Finite Element Method:

Discretizes the physical problem $R(x) = 0$ in elements. In the „weak“ formulation the physical problem is somehow relaxed to $\int_{x_e}^{x_{e+1}} Q_e(x)\, R(x)\, \mathrm{d}x = 0$, with the weight function $Q_e(x)$ for the element e.

Usually one considers the local problem of each element and then combines all of them to the global one. This then typically becomes a set of linear equations [for steady state problems] or a set of ordinary differential equations [time dependent problems].

The mechanism is very general but memory-consuming and not parallelizable.