Numerical Simulation of Lasers

Numerical Simulation of Lasers

Christoph Pflaum

Basic Elements of a Laser

A laser consists mainly of the following three elements :

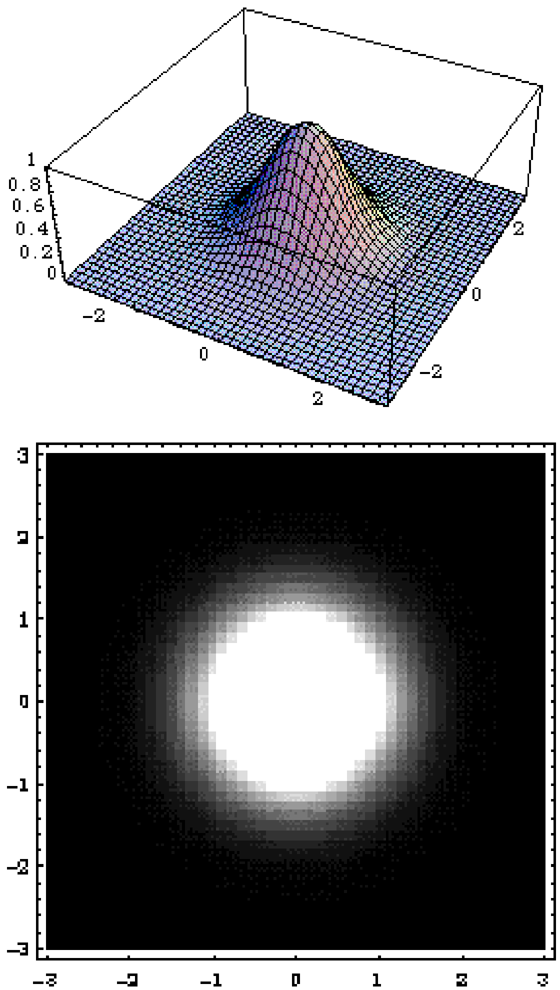
1. Laser medium: collection of atoms, molecules, ions or a semiconductor crystal:
   - gas laser
   - solid state lasers
   - semiconductor lasers
   - fiber laser
2. Pumping process to excite the atoms (molecules) into higher quantum mechanical energy levels.
3. Suitable optical feedback elements
   - as a laser amplifier (one pass of the beam)
   - as a laser oscillator (bounce back and forth of the laser beam)

Model and Simulation

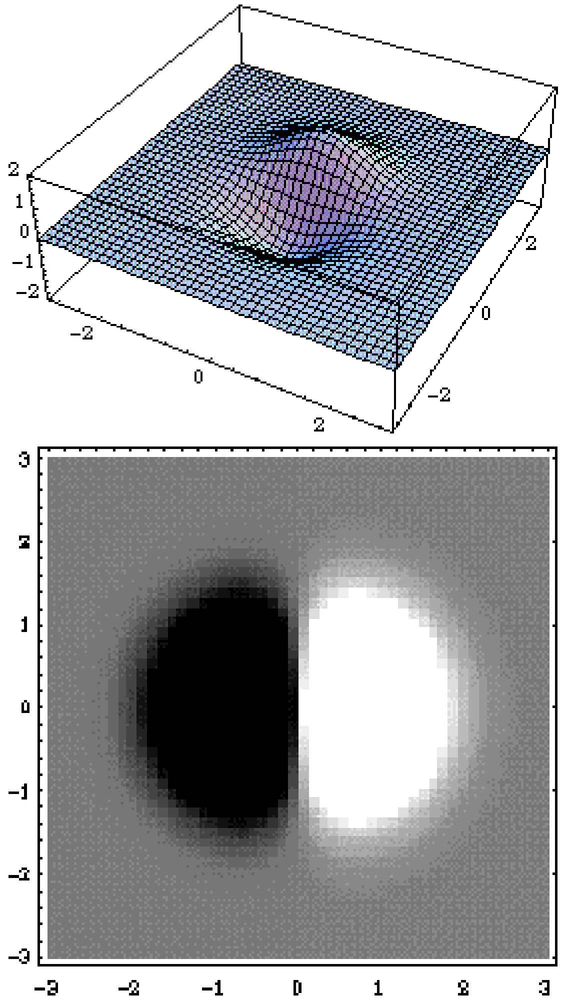
1. Population inversion
2. Amplification of light (electromagnetic radiation) within a certain narrow band of frequencies. The amplification depends on the population inversion.
3. Oscillation: There must be more gain than loss of the beam. Reasons of loss are:
   - loss by medium
   - not accurate construction of the mirrors
   - output
4. Eigenmodes of a laser (e.g. Gauss modes).
   - deformation of the crystal
   - gain, lenses
   - different refraction index

Hermite-Gaussian Modes

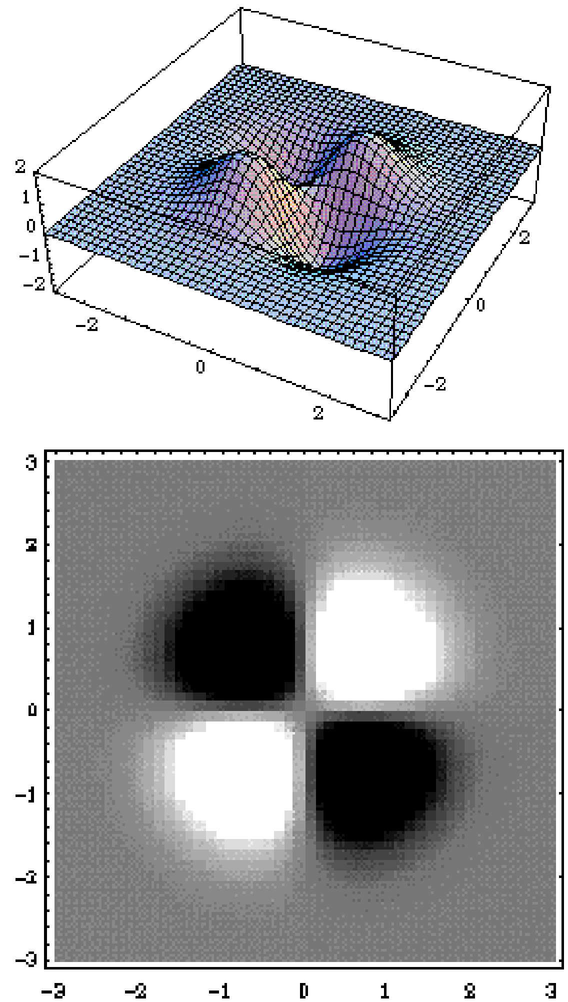
$[0, 0]$ Gaussian



$[0, 1]$ Gaussian



$[1, 1]$ Gaussian



Atomic Energy Levels

Light of a certain wavelength is emitted if a transition between two energy levels $E_2 \to E_1$ takes place “ jump of electrons “ .

Formula 1. *The frequency of the emitted light is*

$$\omega_{21} = \frac{E_2 - E_1}{\hbar}, \tag{1}$$

where

$$\hbar = \frac{h}{2\pi}, \quad h = 6.626 \cdot 10^{-34} Js \quad \text{\textit{Planck's constant.}}$$

Notation for wavelength: $1\mu m = 10000\,\mathring{A}$

Energy which leads to a Transition

Transition from $E_2 \rightarrow E_1$ takes place
only with a little additional energy:

- spontaneous emission: energy from small movements of the atoms
- stimulated emission: energy from absorption

Spontaneous Emission

Let N_i be the number of atoms with energy level E_i.
Within a short period of time a certain percentage of atoms make a transition to a lower level.
This can be described by the following ODE:

$$\left.\frac{dN_2}{dt}\right|_{spon} = -\gamma N_2 = -\frac{N_2}{\tau},$$

where

- γ is called energy-decay rate and
- $\tau = \frac{1}{\gamma}$ is called lifetime.

The solution of this ODE is:

$$N_2(t) = N_2(0)e^{-\frac{t}{\tau}}$$

Stimulated Transition

If an external radiation signal is applied to the atom, then stimulated transitions occur: “ atom reacts like an antenna “. Let $n(t)$ be the photon density of the radiation. Then, there is a constant K such that

$$
\begin{aligned}
\left.\frac{dN_2}{dt}\right|_{stim.upward} &= Kn(t)N_1(t), \quad \text{(absorption)} \\
\left.\frac{dN_2}{dt}\right|_{stim.downward} &= -Kn(t)N_2(t) \quad \text{(stimulated emission)}.
\end{aligned}
$$

This implies:

$$
\left.\frac{dN_2}{dt}\right|_{total} = Kn(t)(N_1(t) - N_2(t)) - \gamma_{21}N_2(t) = -\left.\frac{dN_1}{dt}\right|_{total}.
$$

Energy Transfer of Stimulated Transition

The energy transfer of stimulated transition by a signal is

$$\frac{dU_a}{dt} = Kn(t)(N_1(t) - N_2(t)) \cdot \hbar\omega,$$

where U_a is the energy density.
The energy transfer changes the photon density of the signal by:

$$\frac{dn(t)}{dt} = -K(N_1(t) - N_2(t)) \cdot n(t). \tag{2}$$

- Absorption (attenuation): $N_1(t) > N_2(t)$
- Population inversion: $N_1(t) < N_2(t)$
  $\rightarrow$ net amplification of a signal

Boltzmann's Principle

Theorem 1 (Boltzmann's Principle)**.** *In case of equilibrium the populations N_1 and N_2 depend on the temperature:*

$$\frac{N_2}{N_1} = \exp\left(-\frac{E_2 - E_1}{kT}\right).$$

This implies

$$N_1 - N_2 = N_1\left(1 - e^{-\hbar\frac{\omega}{kT}}\right).$$

Pumping Process

Let

- R_{p0} be the pumping rate (atoms/sec),
- η_p the pumping efficiency such that $R_p = \eta_p R_{p0}$ and
- γ_{ij} the decay rate from level E_i to E_j.

The following formulas describe the pumping process :

$$\begin{aligned} \frac{dN_2}{dt} &= R_p - \gamma_{21} N_2 \\ \frac{dN_1}{dt} &= \gamma_{21} N_2 - \gamma_{10} N_1 \end{aligned}$$

If $\frac{dN_i}{dt} = 0$, then we get

$$N_2 > N_1 \ \text{(population inversion)} \quad \Leftrightarrow \quad \tau_{10} < \tau_{21}$$

Scalar Rate Equations

Let us abbreviate

$$N = N_2 - \frac{g_2 N_1}{g_1}$$

then, the scalar rate equations are

$$\text{(3)} \quad \frac{\partial N}{\partial t} = -\gamma N n \sigma c - \frac{N + N_{tot}(\gamma - 1)}{\tau_f} + R_p(N_{tot} - N)$$

$$\text{(4)} \quad \frac{\partial n}{\partial t} = N n \sigma c - \frac{n}{\tau_c} + S.$$

The unknowns of these equations are

- N: population inversion $N = N_2 - \frac{g_2 N_1}{g_1}$.
- n: photon density

Traveling of an Optical Wave

Let us assume that the optical wave can be modeled by

$$\begin{aligned}\tilde{E}(z,t) &= \exp(j\omega t)E(z)\\ E(z) &= \exp(-jkz+\alpha_m z) = \exp(-jkz)u(z)\\ u(z) &= \exp(\alpha_m z).\end{aligned}$$

This implies that

$$\tilde{E}(z,t) = \exp(j\omega t)\ \cdot\ \exp(-jkz+\alpha_m z)$$

Thus, a constant phase shift is obtained at $\omega t = kz$.
Since $t = z/c$ in vacuum, we get

$$k = \frac{\omega}{c}.$$

(By $k^2 = \mu\epsilon\omega^2$ in Section **??**, we obtain $c = \frac{1}{\sqrt{\mu\epsilon}}$ in vacuum.)

Amplification of the Optical Wave

Now, let us model the optical wave by

$$\begin{aligned}\tilde{E}(z,t) &= \exp(j\omega t)E(z)\\ E(z) &= \exp(-j\omega z/c+\alpha_m z) = \exp(-j\omega z/c)u(z)\\ u(z) &= \exp(\alpha_m z).\end{aligned}$$

Let r_i be the reflection coefficient at the mirrors $M_i, i = 1,2$.
Let L_m be the length of the amplification medium.
Let L be the length of the laser medium. Then, we get

$$r_1 r_2 \exp(2\alpha_m L_m - j2\omega L/c) = 1 \quad \text{and} \quad K(N_2 - N_1) = 2\alpha_m c.$$

Consequences:

$$\begin{aligned}2\omega L/c &\in 2\pi\mathbb{Z} \quad \Rightarrow \text{only certain frequencies!}\\ |r_1 r_2|\exp(2\alpha_m L_m) = 1 &\Rightarrow N_2 - N_1 \geq \frac{c}{K}\frac{1}{2L_M}\ln\left(\left|\frac{1}{r_1}\right|\cdot\left|\frac{1}{r_2}\right|\right)\end{aligned}$$

Scalar Rate Equations

$$\frac{\partial N}{\partial t} = -\gamma N n \sigma c - \frac{N + N_{tot}(\gamma - 1)}{\tau_f} + R_p(N_{tot} - N)$$

$$\frac{\partial n}{\partial t} = N n \sigma c - \frac{n}{\tau_c} + S$$

$$N(0) = N_0 \quad \text{and} \quad n(0) = n_0.$$

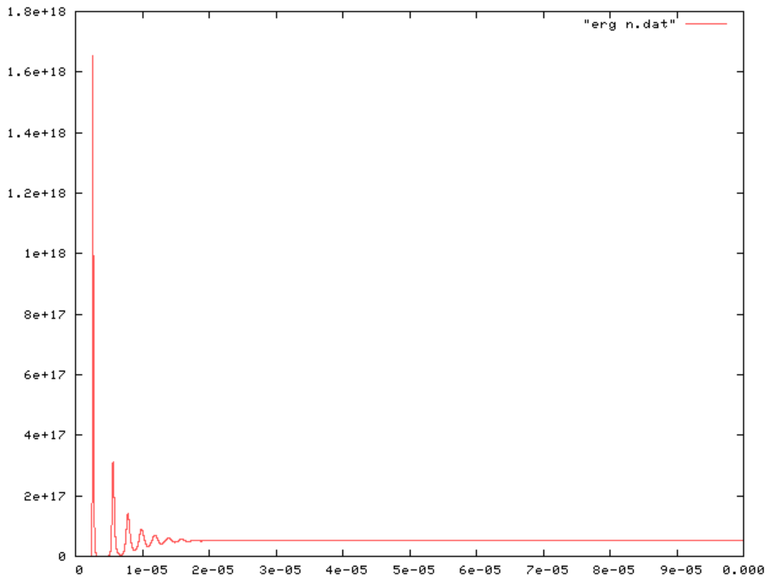
To discretize the unknowns

- N: population inversion $N = N_2 - N_1$.
- n: photon density

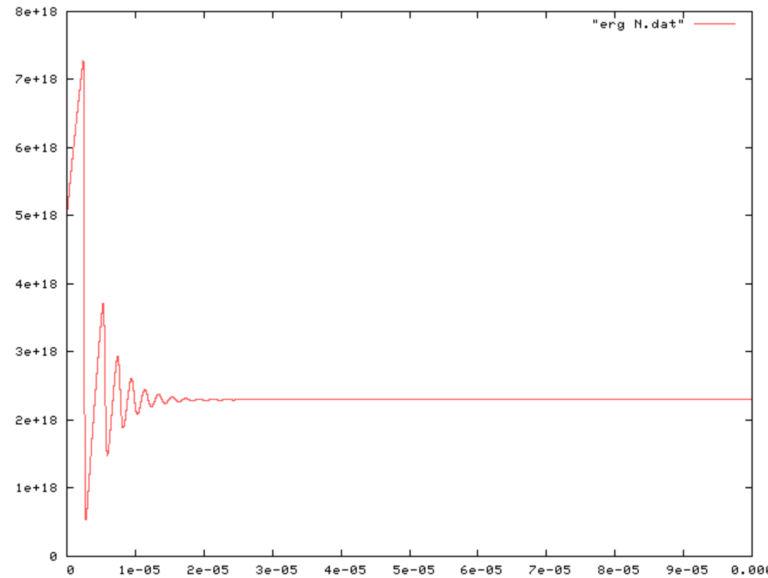
let us use an explicit / implicit Euler discretization with meshsize τ.

Numerical Result

$n(t)$ photon density



$N(t)$ population inversion



The peak of the photon density after switching on the laser resonator leads to the construction of pulsed lasers.

Maxwell's Equations

$$\begin{aligned}
\nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} && \text{Faraday's law} \\
\nabla \times \vec{H} &= \frac{\partial \vec{D}}{\partial t} + \vec{J} && \text{Maxwell-Ampere law} \\
\nabla \cdot \vec{D} &= \rho && \text{Gauss's law} \\
\nabla \cdot \vec{B} &= 0 && \text{Gauss's law - magnetic} \\
\nabla \cdot \vec{J} &= -\frac{\partial \rho}{\partial t} && \text{equation of continuity}
\end{aligned}$$

and constitutive relations:

$$\vec{D} = \epsilon \vec{E}, \quad \vec{B} = \mu \vec{H}, \quad \vec{J} = \sigma \vec{E}$$

Maxwell's Equations

By the assumptions:

- μ is roughly constant.
- $\rho = 0$
- $J = 0$

we get

$$\begin{aligned}
\nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} && \text{Faraday's law} \\
\nabla \times \vec{H} &= \frac{\partial \vec{D}}{\partial t} && \text{Maxwell-Ampere law} \\
\nabla \cdot \vec{D} &= 0 && \text{Gauss's law} \\
\nabla \cdot \vec{B} &= 0 && \text{Gauss's law - magnetic} \\
\vec{D} &= \epsilon \vec{E} \\
\vec{B} &= \mu \vec{H}
\end{aligned}$$

Vector-Helmholtz Equation

Since μ is constant, we get from Maxwell's equations:

$$
\begin{aligned}
\nabla \times \nabla \times \vec{E} &= -\mu \frac{\partial}{\partial t} \nabla \times \vec{H} \\
&= -\mu \frac{\partial}{\partial t} \left(\frac{\partial \vec{D}}{\partial t} + \vec{J} \right).
\end{aligned}
$$

Thus, we get

$$
\nabla \times \nabla \times \vec{E} = -\mu \frac{\partial^2}{\partial t^2} \left(\epsilon \vec{E} \right) - \mu \frac{\partial}{\partial t} \vec{J}.
$$

Now, by $\vec{J} = 0$, we get the vector Helmholtz equation:

$$
\boxed{\nabla \times \nabla \times \vec{E} = -\mu \frac{\partial^2}{\partial t^2} \left(\epsilon \vec{E} \right).}
$$

Assumptions for the Scalar Helmholtz E.

Let us assume the ϵ is constant. Then, we get

$$\epsilon\nabla\cdot\vec{E}=\nabla\cdot\vec{D}=\rho=0.$$

This implies

$$\nabla(\nabla\cdot\vec{E})=0. \tag{5}$$

But, ϵ is not constant! Therefore, we assume (**??**). Then, we get

$$\nabla\times\nabla\times\vec{E}=\nabla(\nabla\cdot\vec{E})-\triangle\vec{E}=-\triangle\vec{E}$$

Furthermore, we assume that

ϵ is constant with respect to time.

Scalar Helmholtz Equation

Now, the vector-Helmholtz equation

$$\nabla \times \nabla \times \vec{E} = -\mu \frac{\partial^2}{\partial t^2} \left(\epsilon \vec{E} \right).$$

and the assumption (**??**) imply

$$-\triangle \vec{E} = -\mu \frac{\partial^2}{\partial t^2} \left(\epsilon \vec{E} \right).$$

Assumption (**??**) is satisfied for the TE-wave (transversal electric wave):

$$\vec{E}(x, y, z) = E(x, y, z) e_x - E(y, x, z) e_y$$

For this wave, we get the scalar Helmholtz equation:

$$-\triangle E = -\mu\epsilon \frac{\partial^2}{\partial t^2} (E). \tag{6}$$

Time Periodic Solution

Let us assume that E is time periodic. This means:

$$E(x, y, z, t) = \exp(i\omega t)E(x, y, z).$$

Inserting in the scalar Helmholtz equation, leads to

$$\boxed{-\triangle E - k^2 E = 0,}$$

where $k^2 = \mu\epsilon\omega^2$.

This is the Helmholtz equation for time periodic solutions.

Paraxial Approximation

Let k_0 be an average value of k. Inserting the ansatz

$$E = e^{-ik_0 z}\Psi(x, y, z)$$

in the scalar Helmholtz equation leads to

$$-\triangle\Psi + 2ik_0\frac{\partial\Psi}{\partial z} + (k_0^2 - k^2)\Psi = 0.$$

In the case that $k = k_0$ is constant, we obtain

$$-\triangle\Psi + 2ik_0\frac{\partial\Psi}{\partial z} = 0.$$

In the paraxial approximation, we neglect the term $\frac{\partial^2\Psi}{\partial z^2}$. This leads to:

$$\boxed{-\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi}{\partial y^2} + 2ik\frac{\partial\Psi}{\partial z} = 0.}$$

Lowest Order Gauss-Mode

To solve the paraxial approximation,

$$\boxed{-\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi}{\partial y^2} + 2ik\frac{\partial\Psi}{\partial z} = 0.}$$

let us make the ansatz

$$\Psi(x, y, z) = A(z)\exp\left(-ik\frac{x^2 + y^2}{2q(z)}\right),$$

where $A(z)$ and $q(z)$ are unknown functions.
This equation leads to the ODE's

$$\frac{\partial q}{\partial z} \quad = \quad 1 \quad \text{and} \quad \frac{\partial A}{\partial z} = -A \cdot \frac{1}{q}.$$

Lowest Order Gauss-Mode

The unique solutions of $\frac{\partial q}{\partial z} = 1$ and $\frac{\partial A}{\partial z} = -A \cdot \frac{1}{q}$ are

- $q(z) = q_0 + z$, where q_0 and z_0 are constants.
- $A(z) = A_0 \frac{q_0}{q(z)}$.

Thus, lowest order Gauss mode is

$$\begin{aligned} E(x,y,z) &= e^{-ikz}\Psi(x,y,z) \\ &= A_0 \frac{q_0}{q_0+z} \exp\left(ik\left(-z - \frac{x^2+y^2}{2(q_0+z)}\right)\right) \end{aligned}$$

Let us normalize the amplitude of this mode by $q_0 A_0 = 1$. Then,

$$\boxed{E(x,y,z) = \frac{1}{q_0+z} \exp\left(-ik\left(z + \frac{x^2+y^2}{2(q_0+z)}\right)\right)}$$

Definition of Spot Size

Definition 1. *The spot size is defined by the radius r such that*

$$e^{-1} = \frac{|E(z,r)|}{|E(z,0)|}$$

Spot Size and Beam Waist

$$E(x,y,z) = \frac{1}{q_0+z}\exp\left(-ik\left(z+\frac{x^2+y^2}{2(q_0+z)}\right)\right)$$

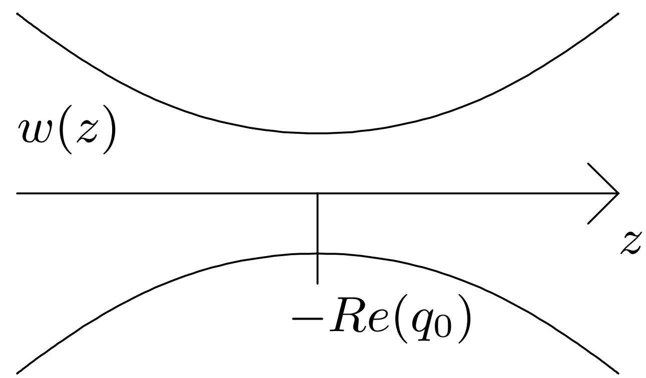
Write

$$\frac{1}{q_0+z} = \frac{1}{q(z)} = \frac{1}{R(z)} - i\frac{\lambda}{\pi w(z)}$$

where

$$R(z) = (\mathsf{Re}(q_0)+z)\left(1+\frac{\mathsf{Im}(q_0)^2}{(\mathsf{Re}(q_0)+z)^2}\right)^2$$

$$w(z) = \frac{\lambda}{\pi}\left(\mathsf{Im}(q_0)+\frac{(\mathsf{Re}(q_0)+z)^2}{\mathsf{Im}(q_0)}\right)$$



Phase shift: $\exp\left(-ik\left(z+\frac{x^2+y^2}{2R(z)}\right)\right)$

Energy of the Beam

A short calculation shows:

$$|q_0 + z|^2 = \frac{\pi |\mathsf{Im}(q_0)|}{\lambda} |w(z)|$$

and:

$$\int_{\mathbb{R}^2} |E|^2 d(xy) = \frac{|A_0 q_0|^2}{|\mathsf{Im}(q_0)|} \frac{\pi}{2} \frac{\pi^2}{\lambda^2 k}$$

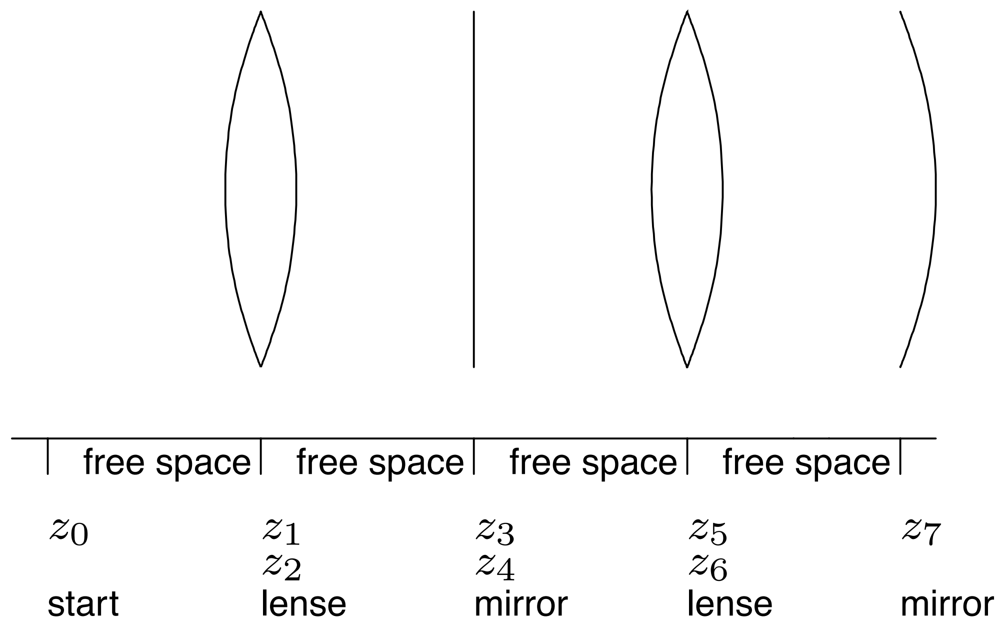
Thus, the energy at a slice $z =$constant is independent of z.

Types of Resonators

There exists several types of resonators . Here, let us study a one way resonator. Other resonators can be transformed to a one way resonator.

Let $\Omega = \Omega_2 \times [0, L]$ be a resonator geometry.
Let us assume that there are n apertures in the resonator.
The start points of these apertures are

$$0 = z_0 \leq z_1 \leq z_2 \leq ... \leq z_n = L.$$



$$E_i(x, y, z) = \mathcal{A}_i \frac{1}{q_i + (z - z_i)} \exp\left(-ik\left((z - z_i) + \frac{x^2 + y^2}{2(q_i + (z - z_i))}\right)\right)$$

where $\mathcal{A}_i := A_i q_i$.

ABCD Matrices

The change of the Gauss-mode is described by ABCD matrices

$$M_i = \begin{pmatrix} A^i & B^i \\ C^i & D^i \end{pmatrix}$$

Then, the beam parameter q_i changes as follows

$$q_i = \frac{A^i q_{i-1} + B^i}{C^i q_{i-1} + D^i} =: M_i[q_{i-1}].$$

Lemma 1.

$$M_{i+1}[M_i[q_{i-1}]] = (M_{i+1}M_i)[q_{i-1}]$$

Ray Optics and ABCD Matrices

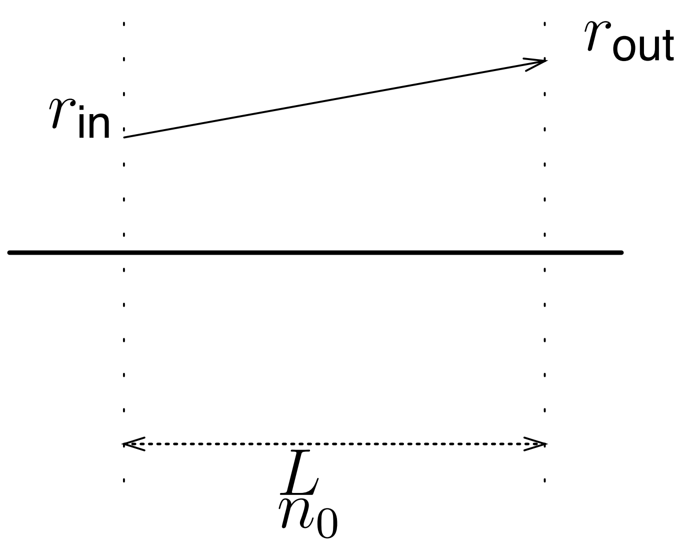
An optical ray can be described by

- the radius $r(z)$ and
- the slope $r'(z)$.

The change of an optical ray is described by

$$\begin{pmatrix} r_{\text{out}} \\ r'_{\text{out}} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} r_{\text{in}} \\ r'_{\text{in}} \end{pmatrix}$$

Example 1 (Ray-matrix of free space)**.**



$$\begin{pmatrix} r_{out} \\ r'_{out} \end{pmatrix} = \begin{pmatrix} 1 & \frac{L}{n_0} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} r_{in} \\ r'_{in} \end{pmatrix}$$

ABCD matrix of free space

Formula 2 (ABCD matrix of free space)**.**

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & z_i - z_{i-1} \\ 0 & 1 \end{pmatrix}$$

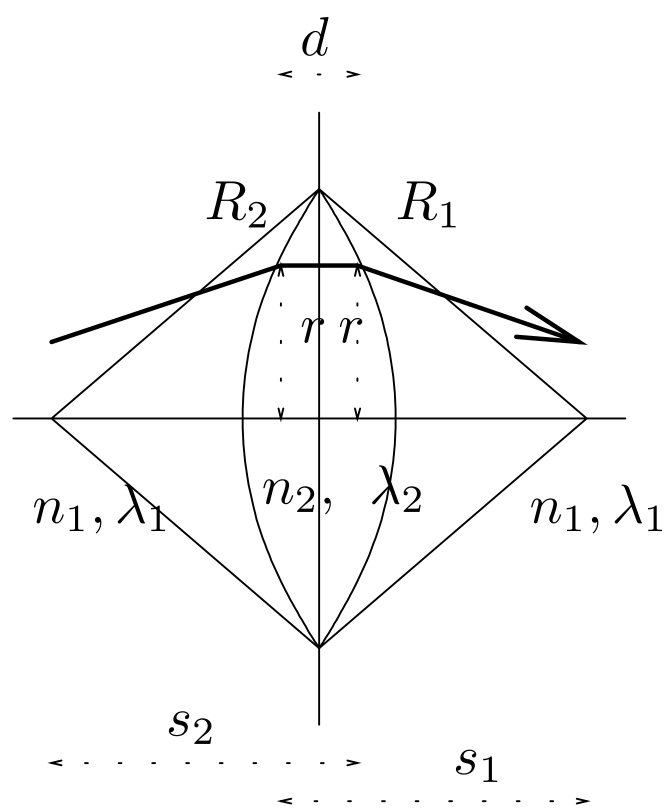
and

$$\mathcal{A}_i = \mathcal{A}_{i-1} \exp(ik(-(z_i - z_{i-1})))$$

ABCD Matrix of a Lense

Formula 3 (ABCD matrix of a lense)**.**

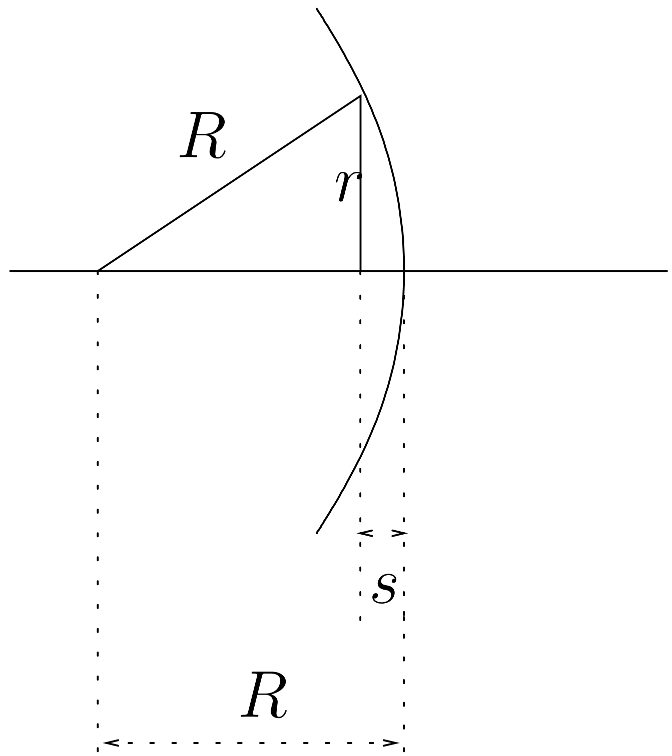
$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\frac{1}{f} & 1 \end{pmatrix} \quad \textit{and} \quad \mathcal{A}_i = \mathcal{A}_{i-1} \frac{1}{1 - \frac{1}{f} q_{i-1}}$$



ABCD Matrix of a Mirror

Formula 4 (ABCD Matrix of a mirror)**.**

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\frac{2}{R} & 1 \end{pmatrix}$$



Other ABCD Matrices

Formula 5 (ABCD Matrix of a Duct)**.**
Let $k = \omega\sqrt{\mu\epsilon}n(x)$*, where* $n(x) = n_0 - \frac{1}{2}n_2x^2$*. Then*

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} \cos(\gamma z) & (n_0\gamma)^{-1}\sin(\gamma z) \\ -(n_0\gamma)\sin(\gamma z) & \cos(\gamma z) \end{pmatrix},$$

where $\gamma^2 = n_2/n_0$*.*

Ray (or Beam) Matrix of the Resonator

Using the ABCD matrix M_i of each aperture on can calculate the ABCD matrix of the whole resonator by

$$M = \prod_{i=1}^{n} M_i =: \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

Lemma 2.

$$\textit{det} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \textit{det}(M) = 1$$

Proof. Observe that for every aperture the corresponding ABCD matrix M_i satisfies det$(M_i) = 1$. □

Let r_0 be a start vector. Consider

$$r_s = M^s r_0$$

Stability Ray of the Resonator

Let q_a, q_b be the eigenvectors of M.
Then,

$$r_s = c_a \lambda_a^s q_a + c_b \lambda_b^s q_b.$$

- Stable Laser: $-1 \leq |m| \leq 1$. Then,

$$r_s = e^{i\Theta n} c_a q_a + e^{-i\Theta n} c_b q_b,$$

  where $\lambda_{a,b} = e^{\substack{+\\-} i\Theta}$.

- Unstable Laser: $|m| \geq 1$. Then,

$$r_s = M^s c_a q_a + M^{-s} c_b q_b,$$

  where $M = \lambda_a$, $\frac{1}{M} = \lambda_b$, $M = m + \sqrt{m^2 - 1}$.

Exact Solution in a Gaussian “Duct”

The refraction index of a Gaussian duct is :

$$k = k_0(1 - \frac{1}{2}n_2 r^2)$$

The paraxial approximation and neglecting the small high order term $\frac{1}{4}n_2^2 r^2$ leads to

$$\triangle_{xy}\Psi - 2ik_0\frac{\partial\Psi}{\partial z} - k_0 n_2 r^2\Psi = 0$$

An exact solution of this equation is:

$$\Psi(x, y, z) = \exp\left(-\frac{x^2 + y^2}{w_1^2} + i\frac{\lambda z}{w_1}\right)$$

where $w_1^2 = 2\frac{1}{k_0\sqrt{n_2}}$ and $\lambda = \frac{2}{k_0}$.

The Guoy Phase Shift

Let us define the Guoy phase shift $\psi(z)$ by:

$$\frac{i|q(z)|}{q(z)} = \exp(i\psi(z)).$$

This implies

$$\tan\psi(z) = \frac{\pi w(z)^2}{R(z)\lambda}.$$

Thus, $\psi(z) = 0$ at the waist of the Gaussian beam. Then, one can show

$$\frac{1}{w_0}\frac{q_0}{q(z)} = \frac{\exp(i(\psi(z) - \psi_0))}{w(z)},$$

where $\psi_0 = \psi(0)$ and $q_0 = q(0)$.

Notation in “Lasers and Electro-Optics”

In this book the spot size at the waist $z = 0$ is:

$$w_D^2(z) \quad = \quad w_0^2 \left(1 + \left(\frac{\lambda z}{\pi w_0^2} \right)^2 \right)$$

By (**??**), we get

$$\begin{aligned} w_D^2(z) = w(z)\Big|_{\mathrm{Re}(q_0)=0} \quad &= \quad \frac{\lambda}{\pi} \left(\mathrm{Im}(q_0) + \frac{(\mathrm{Re}(q_0) + z)^2}{\mathrm{Im}(q_0)} \right) \Big|_{\mathrm{Re}(q_0)=} \\ &\Rightarrow \quad w_0^2 = \frac{\lambda}{\pi} \mathrm{Im}(q_0) \end{aligned}$$

and

$$R(z) = (\mathrm{Re}(q_0) + z) \left(1 + \frac{\mathrm{Im}(q_0)^2}{(\mathrm{Re}(q_0) + z)^2} \right)^2$$

Hermite-Gaussian Modes

$$
\begin{aligned}
\Psi_{m,n} &= \frac{w_0}{w} H_m\left(\sqrt{2}\frac{x}{w}\right) H_n\left(\sqrt{2}\frac{y}{w}\right) \\
&\quad \exp\left(-i(kz-\Phi) - r^2\left(\frac{1}{w^2}+\frac{ik}{2R}\right)\right)
\end{aligned}
$$

where

$$
\Phi(m,n,z) = (m+n+1)\tan^{-1}\left(\frac{\lambda z}{\pi w_0^2}\right)
$$

$$
\begin{aligned}
H_0(x) = 1, \qquad & H_1(x) = x, \\
& H_2(x) = 4x^2 - 2, \ldots \\
& H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}) \qquad n = 0, 1, \ldots
\end{aligned}
$$

The set of these functions forms a basis.

The Laguerre-Gaussian Modes

$$|\Psi_{m,n}| = E_0 \left(\sqrt{2} \frac{r}{w_D} \right)^l L_p^l \left(2 \frac{r^2}{w_D^2} \right) e^{\frac{r^2}{w_D^2}} \cos(l\phi)$$

where r, ϕ are the angle coordinates and

$$L_0^l(x) = 1 \qquad L_1^l(x) = l + 1 - x$$

$$L_2^l(x) = \frac{1}{2}(l+1)(l+2) - (l+2)x + \frac{1}{2}x^2$$

$$L_n(x) = e^x \frac{d^n}{dx^n}(x^n e^{-x}) \qquad n = 0, 1, ...$$

The set of these functions forms a basis.

Thermal lensing

The refraction index $n_c(x)$ of a laser crystal changes by

a) thermal lensing .

b) internal change of the refraction index caused by deformation

c) deformation of the end faces of the laser crystal

Thermal lensing

a) The refraction index of a laser crystal changes by temperature

- Let T_0 be the temperature before heating (refraction index n_0).
- Let T be the temperature caused by the pumping process (refraction index n).

Let η_T be the thermal index gradient.
(Example: $\eta_T = 2.2 \cdot 10^{-6} \cdot\ ^{\circ}C^{-1}$ for Cr^{4+}).
Then,

$$n(x, y, z) = n_0 + \eta_T (T(x, y, z) - T_0)$$

Deformation of a Laser Crystal

Let $\mathcal{B} \subset \mathbb{R}^3$ be the original domain of the laser crystal.
Let $T : \mathcal{B} \to \mathbb{R}^3$ be the mapping of the laser deformation such that

$$\left\{ T(x) + x \;\middle|\; x \in \mathcal{B} \right\}$$

is the deformed domain of the laser crystal.

- Heat and
- deformation

of the crystal lead to a refraction index

$$n_c(x), \qquad x \in \mathcal{B}$$

such that $k_c(x) = \omega\sqrt{\mu\epsilon}n_c(x)$.

Parabolic Fit

Assume that $\mathcal{B} = \mathcal{D} \times]0, L[$, L length of the laser crystal.

b) The parabolic fit of the refraction index is

- Subdivide $]0, L[$ in N intervals of meshsize $h = \frac{L}{N}$.
- Let $\mathcal{D}_h$ be the discretization grid.
- For every $i = 0, ..., N-1$: Find $n_{0,i}, n_{2,i}$ such that:

$$\left\| n_c(x, y, h(i + \frac{1}{2})) - (n_{0,i} - \frac{1}{2} n_{2,i}(x^2 + y^2)) \right\|_{l^2(\mathcal{D}_h)}$$

- Each of the parameters $n_{0,i}, n_{2,i}$ lead to a matrix

$$A_i = \begin{bmatrix} \cos \gamma_i z & n_0 \gamma_i^{-1} \sin \gamma_i z \\ n_0 \gamma_i \sin \gamma_i z & \cos \gamma_i z \end{bmatrix}$$

c) Additionally, perform a parabolic fit of $T(x, y, 0)$ and $T(x, y, L)$.

Beam Propagation Method BPM

The paraxial approximation leads to

$$-\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi}{\partial y^2} + 2ik_0\frac{\partial\Psi}{\partial z} + (k_0^2 - k^2)\Psi = 0.$$

Let us write this equation as follows:

$$2ik_0\frac{\partial\Psi}{\partial z} = \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} - (k_0^2 - k^2)\Psi.$$

Let $\Omega = \mathcal{D}\times]0, L[$, then one can apply

- FE or FD in x, y-direction
- Crank-Nicolson in z-direction.

Beam Propagation Method BPM

Let $\Psi^l(x,y)$ be the approximation of $\Psi(x,y,\tau l)$, where τ is the time step. Then, $\Psi^l(x,y)$ is defined by the equations:

$$
\begin{aligned}
2ik_0 \frac{\Psi^{l+1} - \Psi^l}{\tau} &= \frac{1}{2}\Bigg(\frac{\partial^2 \Psi^{l+1}}{\partial x^2} + \frac{\partial^2 \Psi^{l+1}}{\partial y^2} + (k_0^2 - k^2)\Psi^{l+1} + \\
&\qquad \frac{\partial^2 \Psi^{l}}{\partial x^2} + \frac{\partial^2 \Psi^{l}}{\partial y^2} + (k_0^2 - k^2)\Psi^{l} \Bigg) \\
\Psi^0(x,y) &= \Psi^{\text{initial}}(x,y) \qquad \text{(initial condition)}
\end{aligned}
$$

- Additional boundary conditions are needed .
- Lenses and mirrors can be discretized by a phase shift.

Iteration Method of Fox and Li

Let Ψ^{initial} be an initial condition at the left mirror. By the BPMethod calculate

- the beam configuration at the right mirror and the
- reflected beam configuration $\Psi^{\text{end}} := \mathcal{B}(\Psi^{\text{initial}})$ at the left mirror.

If $\Psi^{\text{initial}} = \Psi^{\text{end}}$, then Ψ^{initial} is an eigenvector Ψ^{eigen} of the BPM operator $\mathcal{B}$.
The iteration method of Fox and Li is a power iteration method for the eigenvalue problem of the BPM operator $\mathcal{B}$.
This means:

$$\Psi^1 = \Psi^{\text{initial}}, \qquad \Psi^{s+1} = \mathcal{B}(\Psi^{\text{initial,s}})$$

$$\Psi^{\text{eigen}} = \lim_{s\to\infty} \Psi^s$$

Weak Formulation of the Helmholtz Equati

Let

$$\mathcal{V} := \{v \in H^1(\Omega)|_{\Gamma_M} = 0\}.$$

Then,

$$\begin{aligned} -\triangle u - k^2 u &= f \\ u|_{\Gamma_M} &= 0, \\ u \cdot ik + \frac{\partial u}{\partial n}|_{\Gamma_R} &= 0 \end{aligned}$$

transforms to:

Problem 1. *Find* $u \in \mathcal{V} = \{v \in H^1(\Omega) \,\big|\, v|_{\Gamma_M} = 0\}$ *such that*

$$\int_\Omega \nabla u \nabla \bar{v} - k^2 u \bar{v}\, d\mu - ik \int_\Gamma \frac{\partial u}{\partial n} \bar{v}\, d\mu = \int_\Omega f \bar{v}\, d\mu \qquad \textit{for every } v \in \mathcal{V}.$$

Weak Formulation of the Helmholtz Equati

Define the bilinear form

$$a(u,v) = \int_\Omega \nabla u \nabla \bar{v} - k^2 u \bar{v} \; d\mu - \int_\Gamma \frac{\partial u}{\partial n} \bar{v} \; d\mu$$

Then, the week form of the Helmholtz equation is transforms to:

Problem 2. *Find* $u \in \mathcal{V} = \{ v \in H^1(\Omega) \; \Big| \; v|_{\Gamma_M} = 0 \}$ *such that*

$$a(u,v) = \int_\Omega f \bar{v} \; d\mu \qquad \text{for every } v \in \mathcal{V}.$$

Properties of $a(u, v)$:

a) The local part of $a(u, v)$ is the bilinear form

$$a^{\text{loc}}(u, v) = \int_\Omega \nabla u \nabla \bar{v} - k^2 u \bar{v} \; d\mu$$

Let k be constant. Then, a^{loc} is not positive definite, since

$$a^{\text{loc}}(e^{\pm i k_1 z}, e^{\pm i k_1 z}) = \begin{cases} > 0 & \text{if } k_1 > k \\ = 0 & \text{if } k_1 = k \\ < 0 & \text{if } k_1 < k \end{cases}$$

Properties of $a(u, v)$:

b) Let k be constant. Then, the functions $e^{\substack{+ \\ -}ikz}$ are contained in the local kernel of a. This means

$$a(e^{\substack{+ \\ -}ikz}, v) = 0 \quad \text{for every } v \in H_0^1(\Omega).$$

Properties of $a(u,v)$:

c) The bilinear form $a(u,v)$ is H^1-coercive. This means that there exist $c, C > 0$ such that

$$\text{Re}(a(u,u)) + C\|u\|_{L^2}^2 \geq c\|u\|_{H^1}^2 \qquad \forall u \in H^1(\Omega)$$

Properties of $a(u, v)$:

d) The problem

Find $u \in \mathcal{V}$ such that

$$a(u, v) = 0 \qquad \text{for every } v \in \mathcal{V}$$

has the unique solution $u = 0$, if $k > 0$.

Properties of $a(u, v)$:

d) The problem

Find $u \in \mathcal{V}$ such that

$$a(u, v) = 0 \qquad \text{for every } v \in \mathcal{V}$$

has the unique solution $u = 0$, if $k > 0$.

Boundary Conditions

Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$ be an open d-dimensional open bounded domain. Consider

$$-\triangle u - k^2 u = 0$$

The rays $\exp(ik\ \vec{m} \cdot x)$ are solutions of this equation, where $\vec{m} = 1$.

Boundary Conditions in 1D

First, let us consider the 1D case $d = 1$ and $\Omega =]0,1[$. Then

$$\exp(ikz) \quad \text{and} \quad \exp(-ikz)$$

are solutions of $-\frac{\partial^2 u}{\partial z^2} - k^2 u = 0$.
Let us assume that the reflection of the ray $\exp(-ikz)$ at the point 0 is $\alpha \exp(ikz)$.
This means we need a boundary condition at 0 with solution

$$u(x) = \exp(-ikz) + \alpha \exp(ikz).$$

A suitable boundary condition is

$$u|_{z=0}(1-\alpha)ik + (1+\alpha)\frac{\partial u}{\partial z}|_{z=0} = 0.$$

Simple Boundary Conditions

- *Reflecting boundary condition:*

$$u\big|_{z=0} = 0$$

- *Non-reflecting boundary condition:*

$$u\big|_{z=0} ik + \frac{\partial u}{\partial \vec{n}}\big|_{z=0} = 0.$$

Non-Reflecting Boundary Condition in 2D,3

- Observe that

$$\lim_{x\to-\infty} \exp(-i(k+i\alpha)\,\vec{m}\cdot x) = 0,$$

where $\alpha > 0$. This leads to the concept:

- Extend the PDE outside of the domain.
- Add an adsorbtion coefficient α outside of the domain.
- Put homogenous Dirichlet boundary conditions at a certain distance for away from the boundary.

Difficulties of a Pure FE Discretization

- One difficulty is the large number of discretization grid points which are needed in case of long resonators. Difficulties occur, if $1cm = L >> 5\lambda = 10\mu m$. Then, more than $20 * 1000 = 20000$ grid points are needed only in z-direction.
- The second difficulty is that a is not symmetric positive definite and the resulting linear equation system cannot efficiently be solved by multigrid or any other standard iterative solver.
- There exist several eigenvectors with eigenvalues close to each other.
- A very accurate discretization of the non-reflecting boundary condition is needed.

Modeling the Wave in a Resonator

Let us model the wave $E(x, y, z)$ in a one way resonator by the following equations:

$$\begin{aligned} -\Delta u + 2ik_f \frac{\partial u}{\partial z} + k_s(2k_f - k_s)u &= \xi u \\ E(x, y, z) &= \exp\left[-i(k_f - \varepsilon)z\right] u(x, y, z) \\ 2\varepsilon k_f &= \xi \end{aligned}$$

Modeling the Wave in a Resonator

Let us assume that $\Phi \subset \mathbb{R}^2$ is a bounded and connected domain with a piecewise smooth boundary and let

$$\Omega = \Phi \times]0, L[,$$

where $L > 0$. Let us subdivide the boundaries of Ω by

$$\Gamma_0 := \Phi \times \{0\}, \quad \Gamma_L := \Phi \times \{L\} \text{ and } \Gamma_r := \partial\Omega \setminus (\Gamma_0 \cup \Gamma_L).$$

For reasons of simplicity, let us additionally assume that we choose k_f such that

(7) $$exp[jLk_f] = 1.$$

Two-Wave Ansatz for Resonator Modeling

Let us model the resonator by a forward wave E_r and the backward wave E_l such that

$$E = E_r + E_l,$$

where each of these waves satisfy the Helmholtz equation .
This leads to the eigenvalue problem:

$$\begin{aligned} -\Delta u_r + 2jk_f \frac{\partial u_r}{\partial z} + (k_f^2 - k^2)u_r &= \xi u_r, \\ -\Delta u_l - 2jk_f \frac{\partial u_l}{\partial z} + (k_f^2 - k^2)u_l &= \xi u_l, \end{aligned} \tag{8}$$

where

$$\begin{aligned} E_r(x,y,z) &= \exp\left[-jk_f z\right] u_r(x,y,z), \\ E_l(x,y,z) &= \exp\left[-jk_f (L-z)\right] u_l(x,y,z), \end{aligned}$$

Boundary Conditions for Two-Wave Ansat

To satisfy the boundary conditions (**??**) and (**??**), we need the boundary conditions

$$
\begin{aligned}
&(9) & u_r + u_l\Big|_{\Gamma_0\cup\Gamma_L} &= 0,\\
&(10) & \frac{\partial u_r}{\partial \vec{n}} - jC_b u_r\Big|_{\Gamma_r} &= 0,\\
&(11) & \frac{\partial u_l}{\partial \vec{n}} - jC_b u_l\Big|_{\Gamma_r} &= 0.
\end{aligned}
$$

Observe that (**??**) is needed to obtain $E_r + E_l\Big|_{\Gamma_0\cup\Gamma_L} = 0$ from $u_r + u_l\Big|_{\Gamma_0\cup\Gamma_L} = 0$.

To obtain a system of equations with enough equations, we additionally need the boundary condition

$$
(12) \qquad \frac{\partial u_r}{\partial z} - \frac{\partial u_l}{\partial z}\Big|_{\Gamma_0\cup\Gamma_L} = 0.
$$

Weak Formulation

Let us define

$$\vec{\mathcal{H}}^1 = \left\{ (u_r, u_l) \in H^1(\Omega) \times H^1(\Omega) \;\middle|\; u_r + u_l\big|_{\Gamma_0} = 0,\; u_r + u_l|_{\Gamma_L} = 0 \right\}.$$

$$\begin{aligned}
&\vec{a}((u_r, u_l), (v_r, v_l)) = \\
&\quad = \int_\Omega \left(\nabla u_r \nabla \bar{v}_r + (k_f^2 - k^2) u_r \bar{v}_r + 2jk_f \frac{\partial u_r}{\partial z} \bar{v}_r \right) - jC_b \int_{\Gamma_r} u_r \bar{v}_r \\
&\qquad + \int_\Omega \left(\nabla u_l \nabla \bar{v}_l + (k_f^2 - k^2) u_l \bar{v}_l - 2jk_f \frac{\partial u_l}{\partial z} \bar{v}_l \right) - jC_b \int_{\Gamma_r} u_l \bar{v}_l,
\end{aligned}$$

where we assume that $k \in L^\infty(\Omega)$.

Now, the weak formulation is:

Find $\vec{u} = (u_r, u_l) \in \vec{\mathcal{H}}^1$ and $\xi \in \mathbb{C}$ such that

$$\vec{a}(\vec{u}, \vec{v}) = \xi \int_\Omega u_r \overline{v_r} + u_l \overline{v_l} \qquad \forall \vec{v} = (v_r, v_l) \in \vec{\mathcal{H}}^1.$$

Properties of a

Lemma 3. *Let* $C_b = 0$. *Then,* $\vec{a}(\vec{u}, \vec{v})$ *is symmetric.*

But $\vec{a}(\vec{u}, \vec{v})$ is not positive definite.

Trilinear Finite Elements

$$\Omega_h := \{(ih_x, jh_y, kh_z) \mid i,j = -N_x, ..., N_x \text{ and } k = 0, ..., N_z\},$$

where we set $h = (h_x, h_y, h_z)$. Furthermore, we obtain the following set of cells

$$\begin{aligned} \tau := \quad \{ \quad & [ih_x, (i+1)h_x] \times [ih_y, (i+1)h_y] \times [ih_z, (i+1)h_z] | \\ & i,j = -N_x, ..., N_x - 1 \quad \text{and} \quad k = -N_z, ..., N_z - 1\}. \end{aligned}$$

Let us define the space of trilinear finite elements by

$$\begin{aligned} V_h := \Big\{ u \in \mathcal{C}(\Omega) \quad \Big| \quad & \forall T \in \tau : \quad \exists c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8 \in \mathbb{C} : \\ & u(x,y,z)|_T = c_1 + c_2 x + c_3 y + c_4 z + \\ & c_5 xy + c_6 yz + c_7 xy + c_8 xyz \Big\} \end{aligned}$$

Two Wave Finite Element Space

Let us define the finite element space

$$\vec{V}_h := \left\{ (u_{h,r}, u_{h,l}) \in V_h \times V_h \;\middle|\; u_{h,r} + u_{h,l}\big|_{\Gamma_0} = 0,\; u_{h,r} + u_{h,l}|_{\Gamma_L} = 0 \right\} \subset \vec{\mathcal{H}}^1$$

An unstable FE-discretization is:

Find $\vec{u}_h \in \vec{V}_h$ such that

$$\vec{a}(\vec{u}_h, \vec{v}_h) = \int_\Omega \vec{f} \vec{v} d \quad \forall \vec{v}_h \in \vec{V}_h$$

The resulting linear equation system is difficult to solve.

FE-Theory for Sym. Positive Definite S.F.

Theorem 2. *Let a be a continuous symmetric positive definite sesquilinear form on a Hilbert space V, V_h a closed subspace and $f \in V'$. Furthermore, let $u \in V$ and $u_h \in V_h$ such that*

$$\begin{aligned} a(u, v) &= f(v) \quad \forall v \in V \\ a(u_h, v_h) &= f(v_h) \quad \forall v_h \in V_h \end{aligned}$$

Then,

$$\|u - u_h\|_E \leq \inf_{v_h \in V_h} \|u - v_h\|_E,$$

where $\|.\|_E$ is the norm corresponding to a.

FE-Theory for Positive Definite S.F.

Theorem 3. *Let a be a continuous positive definite sesquilinear form on a Hilbert space V, V_h a closed subspace of V and $f \in V'$. Furthermore, let us assume that a is V-elliptic. This means that there is a constant $\alpha > 0$ such that*

$$|a(u,u)| \geq \alpha \|u\|^2 \quad \forall u \in V.$$

The continuity of a implies that there is a constant C such that

$$a(u,v) \leq C\|u\|\|v\| \quad \forall u,v \in V.$$

Furthermore, let $u \in V$ and $u_h \in V_h$ such that

$$a(u,v) = f(v) \quad \forall v \in V, \qquad a(u_h, v_h) = f(v_h) \quad \forall v_h \in V_h.$$

Then,

$$\|u - u_h\| \leq \frac{C}{\alpha} \inf_{v_h \in V_h} \|u - v_h\|.$$

Streamline-Diffusion Discretization

(13) $$-\Delta u + 2ik_f \frac{\partial u}{\partial z} + k_s(2k_f - k_s)u = f \qquad \text{on } \mathcal{B}.$$

Let us extend the subdivision τ of Ω to a subdivision $\tau_{\mathcal{B}}$ of $\mathcal{B}$ by using the same meshsize. Furthermore, let $V_{h,\mathcal{B}}$ be the corresponding finite element space of trilinear functions.

Discretization: Find $u_h \in V_{h,\mathcal{B}}$ such that

$$\begin{aligned} -C_b \int_{\partial\mathcal{B}} u_h \bar{v}_h \quad & + \\ + \int_{\mathcal{B}} \nabla u_h \nabla \bar{v}_h + 2ik_f \frac{\partial u_h}{\partial z}(\bar{v}_h + h\rho \frac{\partial}{\partial z}\bar{v}_h) \quad & + \\ k_s(2k_f - k_s)u_h(\bar{v}_h + h\rho\frac{\partial}{\partial z}\bar{v}_h)\, d \quad & = \quad \int_T f(\bar{v}_h + h\rho\frac{\partial}{\partial z}\bar{v}_h)\, d \end{aligned}$$

$\forall v_h \in V_{h,\mathcal{B}}$.

Streamline-Diffusion Discretization

An stable FE-discretization is:

Find $\vec{u}_h \in \vec{V}_h$ such that

$$
\begin{aligned}
\vec{a}(\vec{u}_h, \vec{v}_h) \quad & + \quad \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,r}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,r}}}{\partial \mathbf{z}} \; d \\
& + \quad \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,l}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,l}}}{\partial \mathbf{z}} \; d \\
& = \quad \int_{\Omega} \vec{f} \vec{v}_h d \\
& + \quad h\rho \left(\int_{\Omega} f_r \frac{\partial}{\partial z} \bar{v}_{h,r} \; d - \int_{\Omega} f_l \frac{\partial}{\partial z} \bar{v}_{h,l} \; d \right) \quad \forall \vec{v}_h \in \vec{V}_h
\end{aligned}
$$

We call this discretization streamline-diffusion discretization. However, there are no streamlines. In case of a convection-diffusion equation, this discretization converges with $O(h^2)$.

Ellipticity

The sesquilinear form of the streamline-diffusion discretization is

$$\begin{aligned}\vec{a}_h(\vec{u}_h,\vec{v}_h) &= \vec{a}(\vec{u}_h,\vec{v}_h) \\ &+ \mathbf{h}\rho\int_{\boldsymbol{\Omega}} \mathbf{2ik_f}\frac{\partial \mathbf{u_{h,r}}}{\partial \mathbf{z}}\frac{\partial \bar{\mathbf{v}}_{\mathbf{h,r}}}{\partial \mathbf{z}}\,\mathbf{d} + \mathbf{h}\rho\int_{\boldsymbol{\Omega}} \mathbf{2ik_f}\frac{\partial \mathbf{u_{h,l}}}{\partial \mathbf{z}}\frac{\partial \bar{\mathbf{v}}_{\mathbf{h,l}}}{\partial \mathbf{z}}\,\mathbf{d}\end{aligned}$$

Lemma 4. *For every $\vec{v}_h \in \vec{V}_h$ the following inequality holds:*

$$|\vec{a}_h(\vec{v}_h,\vec{v}_h)| \geq hk_f\rho\left\|\frac{\partial \vec{v}_h}{\partial z}\right\|^2.$$

A Smoothness Result

$$
\begin{aligned}
\vec{a}_h(\vec{u}_h, \vec{v}_h) &= \vec{a}(\vec{u}_h, \vec{v}_h) \\
&+ \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,r}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,r}}}{\partial \mathbf{z}}\, \mathbf{d} + \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,l}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,l}}}{\partial \mathbf{z}}\, \mathbf{d}
\end{aligned}
$$

Lemma 5. *Let $\vec{u}_h^c \in \vec{\mathcal{H}}^1$ such that:*

$$\vec{a}_h(\vec{u}_h^c, \vec{v}) = \int_\Omega \vec{f}\vec{v}\, d \quad \forall \vec{v} \in \vec{\mathcal{H}}^1.$$

Then,

$$\left\| \frac{\partial^2 \vec{u}_h^c}{\partial z^2} \right\|_2 \leq \frac{C}{h\rho k_f} \|\vec{f}\|_{L^2}.$$

FE-Theory for Positive Definite S.F.

Since $\vec{a}_h$ satisfies the Garding inequality, one can prove the following convergence theorem:

Theorem 4. *Assume $\vec{f} = (f_r, f_l) \in L^2(\Omega)^2$. Let $\vec{u} = (u_r, u_l) \in \vec{\mathcal{H}}^1$ such that*

$$\vec{a}(\vec{u}, \vec{v}) \;=\; \int_\Omega f_r \overline{v_r} + f_l \overline{v_l} \qquad \forall \vec{v} = (v_r, v_l) \in \vec{\mathcal{H}}^1.$$

and $\vec{u}_h = (u_{r,h}, u_{l,h}) \in \vec{V}_h$ such that

$$\vec{a}_h(\vec{u}_h, \vec{v}_h) \;=\; \int_\Omega f_r \overline{v_r} + f_l \overline{v_l} \qquad \forall \vec{v}_h = (v_r, v_l) \in \vec{V}_h.$$

Then, $\vec{u}_h$ converges to $\vec{u}$.

A Symmetry Consideration

Instead of

$$\begin{aligned}\vec{a}_h(\vec{u}_h, \vec{v}_h) &:= \vec{a}(\vec{u}_h, \vec{v}_h) \\ &+ \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,r}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,r}}}{\partial \mathbf{z}}\, \mathbf{d} + \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,l}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,l}}}{\partial \mathbf{z}}\, \mathbf{d}\end{aligned}$$

one can define

$$\begin{aligned}\vec{a}_h(\vec{u}_h, \vec{v}_h) &:= \vec{a}(\vec{u}_h, \vec{v}_h) \\ &- \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,r}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,r}}}{\partial \mathbf{z}}\, \mathbf{d} - \mathbf{h}\rho \int_{\mathbf{\Omega}} \mathbf{2ik_f} \frac{\partial \mathbf{u_{h,l}}}{\partial \mathbf{z}} \frac{\partial \bar{\mathbf{v}}_{\mathbf{h,l}}}{\partial \mathbf{z}}\, \mathbf{d}\end{aligned}$$

Then, the meaning of $u_{h,r}$ and $u_{h,l}$ changes and the meaning of t and $-t$ in the ansatz

$$E(x, y, z, t) = \exp(i\omega t) E(x, y, z).$$

Streamline-Diffusion Discretization in 1D

In 1D the sesquilinear form

$$2ik_f \int_0^1 \frac{\partial u_h}{\partial z} \bar{v}_h \; d + h\rho \frac{\partial u_h}{\partial z} \frac{\partial \bar{v}_h}{\partial z} \; d$$

leads to the stencil

$$ik_f \frac{1}{2} (-1 \;\; 0 \;\; 1) + ik_f \frac{1}{h} \rho h \, (-1 \;\; 2 \;\; -1) = ik_f \, (-1 \;\; 1 \;\; 0)$$

for $\rho = \frac{1}{2}$. This is the FD upwind discretization. An exact solver for the resulting equation system is a Gauss-Seidel relaxation from left to right.

Iterative Solver

Hackbusch's rule: Consider a singular perturbed problem with parameter $\epsilon \to \epsilon_0$. Then, construct an iterative solver such that this solver is an exact solver for ϵ_0 (usually $\epsilon_0 = 0$).

The transformed one way resonator equation is:

$$-\epsilon \Delta u + 2i \frac{\partial u}{\partial z} + \epsilon k_s (2k_f - k_s) u = \epsilon \xi u$$

where $\epsilon = \frac{1}{k_f}$. Then, in 1D, the streamline diffusion discretization stencil for $\epsilon \to 0$ is

$$i \begin{pmatrix} -1 & 1 & 0 \end{pmatrix}$$

An exact solver for the corresponding equation system with suitable boundary conditions is a relaxation from left to right. Thus, we used a relaxation from left to right as a preconditioner for GMRES.

Numerical Results

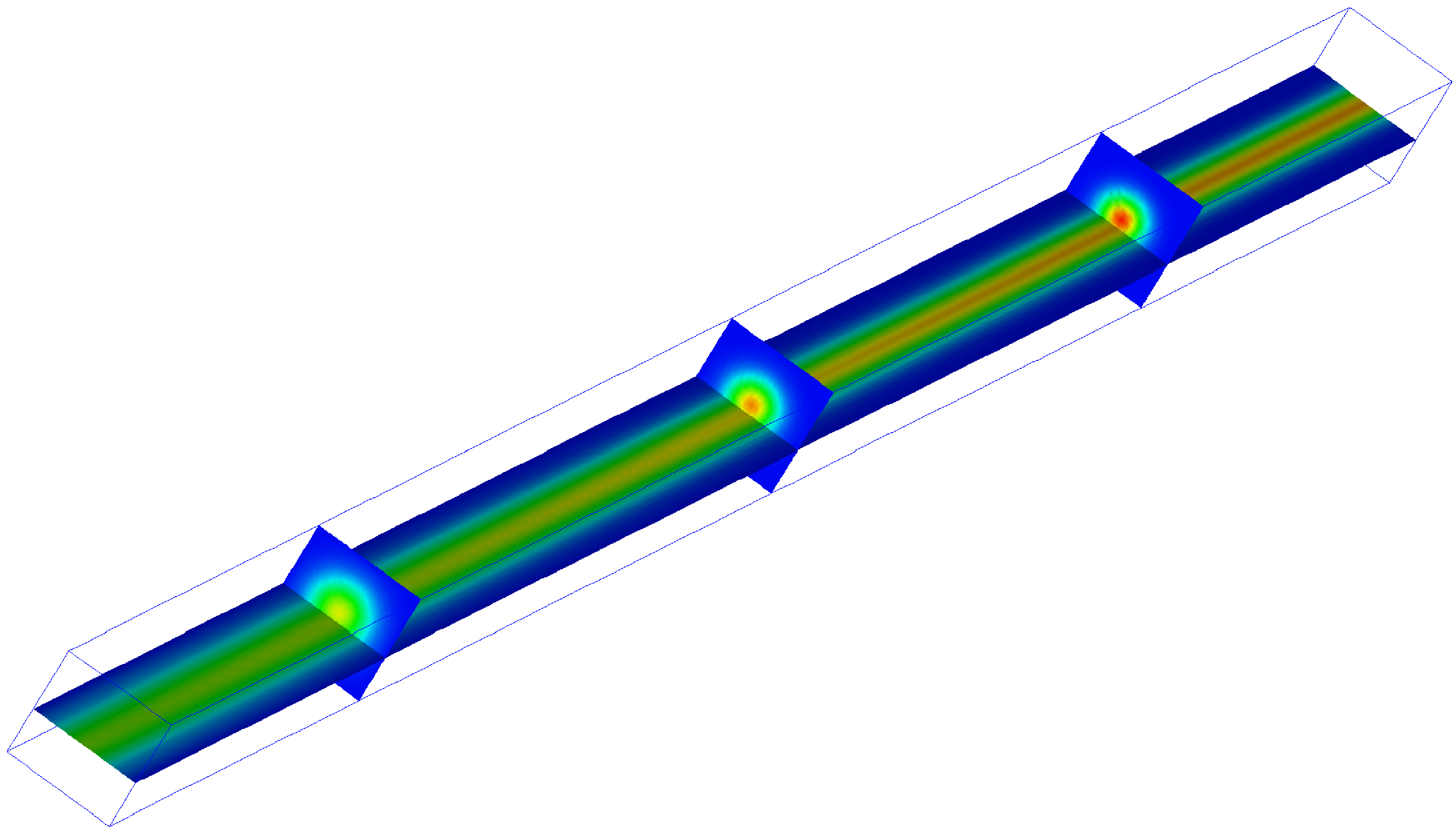


Figure 1: Gauss-Mode by FE

Numerical Results

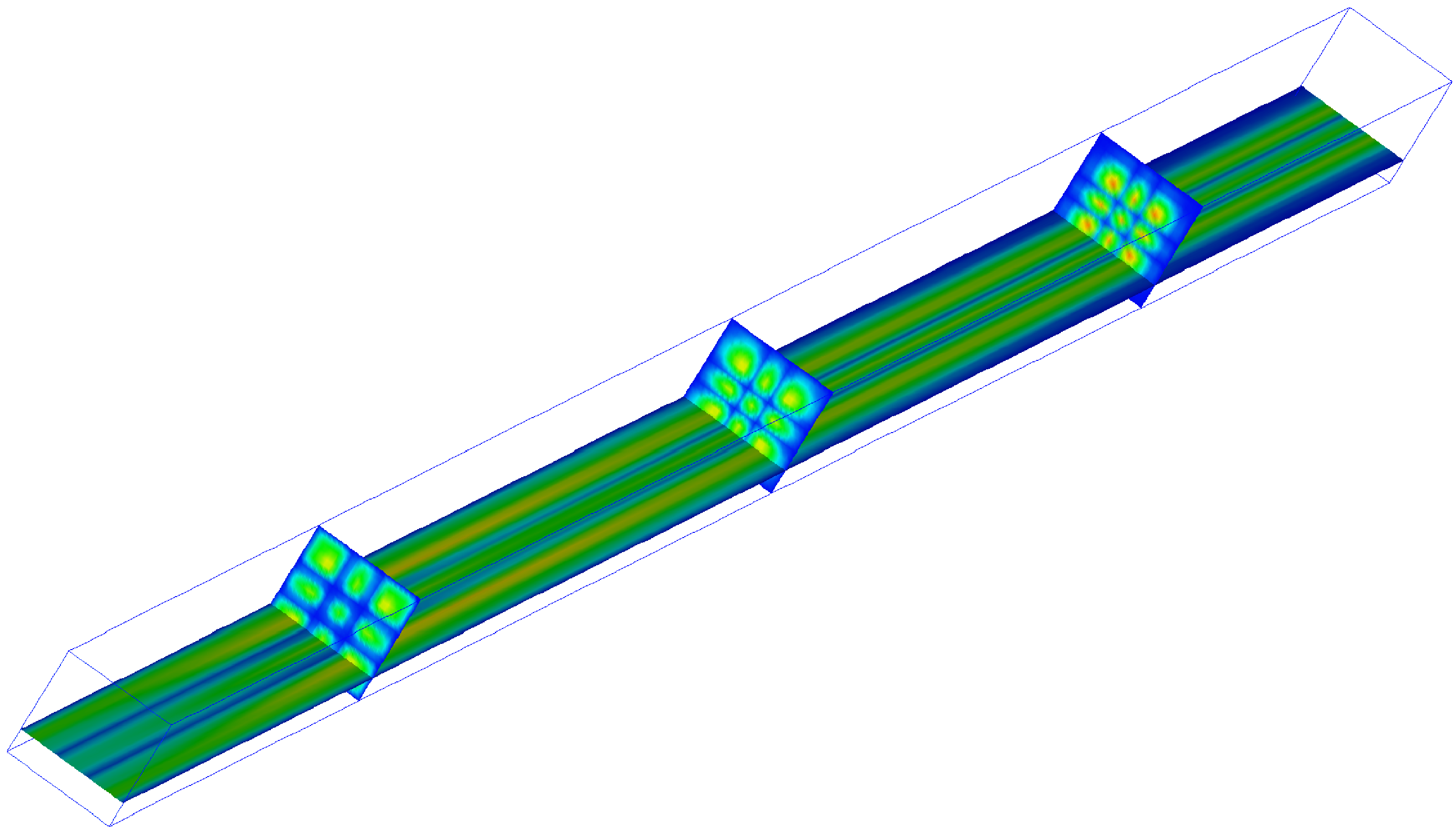


Figure 2: Gauss-Mode by FE

Modeling Optical Apparatuses

Here: One-way resonator with a lense or an interface at the point l_0 with $0 < l_0 < L$. Let us write

$\Omega_a = \Psi \times [0, l_0] \subset \mathcal{B}$ and $\Omega_b = \Psi \times [l_0, L] \subset \mathcal{B}. \Psi_I = \Psi \times \{l_0\}$.

Then, the ansatz

$$E(x, y, z) = \exp\left[-ik_f z\right] u(x, y, z)$$

is not appropriate. Instead, we use the ansatz

$$E(x, y, z) = u(x, y, z) \begin{cases} \exp\left[-ik_{f,\Omega_a} z\right] u(x, y, z) & \text{for } z < l_0 \\ \exp\left[-ik_{f,\Omega_b} z\right] u(x, y, z) & \text{for } z > l_0. \end{cases},$$

where $k_{f,a}$ is an average value of k_f in Ω_a and $k_{f,b}$ is an average value of k_f in Ω_b.

Modeling Optical Apparatuses

$$
\begin{aligned}
a_{\Xi}(u,v) &:= \int_{\Xi} \nabla u \nabla \bar{v} + 2ik_{f,\Xi}\frac{\partial u}{\partial z}\bar{v} + k_s(2k_{f,\Xi} - k_s)u\bar{v}\ d \\
a(u,v) &= a_{\Omega_a}(u,v) + a_{\Omega_b}(u,v).
\end{aligned}
$$

Phase shift of the apparatuses: $\varphi(x,y)$.

Then, let us define the space

$$
\mathcal{H}_{ab} = \Big\{ u \in L^2(\mathcal{B}) \ \Big| \ u|_{\Omega_a} \in H^1(\Omega_a), \quad u|_{\Omega_b} \in H^1(\Omega_b) \quad \text{and} \quad u|_{\Psi_I,\Omega_a} \cdot \varphi = u|_{\Psi_I,\Omega_b} \Big\}.
$$

Find $u \in \mathcal{H}_{ab}$ such that

$$
a(u,v) = \int_{\mathcal{B}} u\bar{v}\ d \quad \forall v \in \mathcal{H}_{ab}.
$$

Gain and Absorption

To simulate gain and absorption in the Helmholtz equation

$$-\triangle u - k^2 u = 0$$

we apply the formula

$$k^2 = \omega^2 \mu\epsilon + j2\omega\sqrt{\mu\epsilon}\alpha.$$

By rate equations, we obtain $K = \sigma c$ and

$$\alpha_{\text{gain}} = \ 1/2\ \sigma N$$

Thus, we get

$$\begin{aligned} k^2 &= \omega^2 \mu\epsilon + j\omega\sqrt{\mu\epsilon}(\sigma N - 2\alpha_{\text{absorption}}) \\ &= \omega^2 \mu\epsilon + j\omega\sqrt{\mu\epsilon}(\sigma N - \frac{1}{\tau_c}). \end{aligned}$$

Time-Dependent Behavior

Using the ansatz

$$E(x,y,z,t) = \exp(i\omega t)(E_r(x,y,z,t) + E_l(x,y,z,t))$$

we obtain

$$\begin{aligned}
\mu\epsilon\frac{\partial^2 u_r}{\partial t^2} + i\mu\epsilon\omega\frac{\partial u_r}{\partial t} &= \Delta u_r - 2jk_f\frac{\partial u_r}{\partial z} - (k_f^2 - k^2)u_r, \\
\mu\epsilon\frac{\partial^2 u_l}{\partial t^2} + i\mu\epsilon\omega\frac{\partial u_l}{\partial t} &= \Delta u_l + 2jk_f\frac{\partial u_l}{\partial z} - (k_f^2 - k^2)u_l, \\
\frac{\partial N}{\partial t} &= -\gamma N n\sigma c - \frac{N + N_{tot}(\gamma - 1)}{\tau_f} + R_p(N_{tot} - N) \\
k^2 &= \omega^2\mu\epsilon + j\omega\sqrt{\mu\epsilon}(\sigma N - \frac{1}{\tau_c}) \\
n &= \frac{\epsilon}{2\hbar\omega}|E|^2 \\
|E|^2 &= |u_r|^2 + |u_l|^2.
\end{aligned}$$

Weak Formulation for the Maxwell Equati

The time-periodic vector Helmholtz equation is

$$\nabla \times \nabla \times \vec{E} - k^2 \vec{E} = \vec{f}.$$

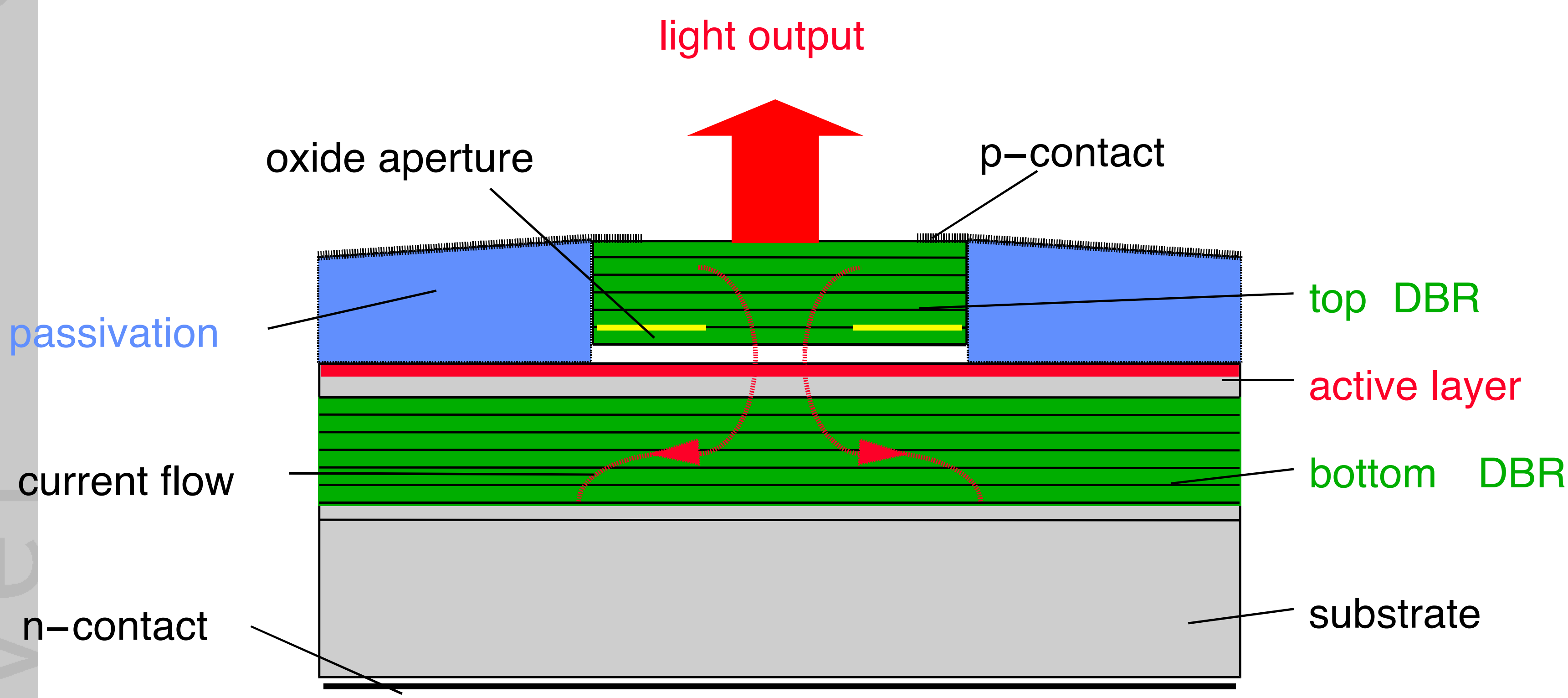
The bilinear form of the weak formulation is positive definite:

$$a(\vec{E}, \vec{W}) = \int_\Omega \nabla \times \vec{E} \cdot \nabla \times \bar{\vec{W}} + k^2 \vec{E} \bar{\vec{W}} \; d(x, y, z)$$

Then, we obtain

$$\begin{aligned} a(e^{-ikz}\vec{u}, e^{-ikz}\vec{w}) \quad = \quad & \int_\Omega \nabla \times \vec{u} \cdot \nabla \times \bar{\vec{v}} + (k^2 - k_f^2) u_z \bar{v}_z \\ & -ik_f 2 \left(\frac{\partial u_z}{\partial y} - \frac{\partial u_y}{\partial z} \right) \bar{v}_y + (k^2 - k_f^2) u_y \bar{v}_y \\ & -ik_f 2 \left(\frac{\partial u_z}{\partial x} - \frac{\partial u_x}{\partial z} \right) \bar{v}_x + (k^2 - k_f^2) u_x \bar{v}_x \; d(x, y, z) \end{aligned}$$

VCSEL (Vertical Cavity Surface Emitting Laser)



DFB Laser (Distributed Feedback Laser)

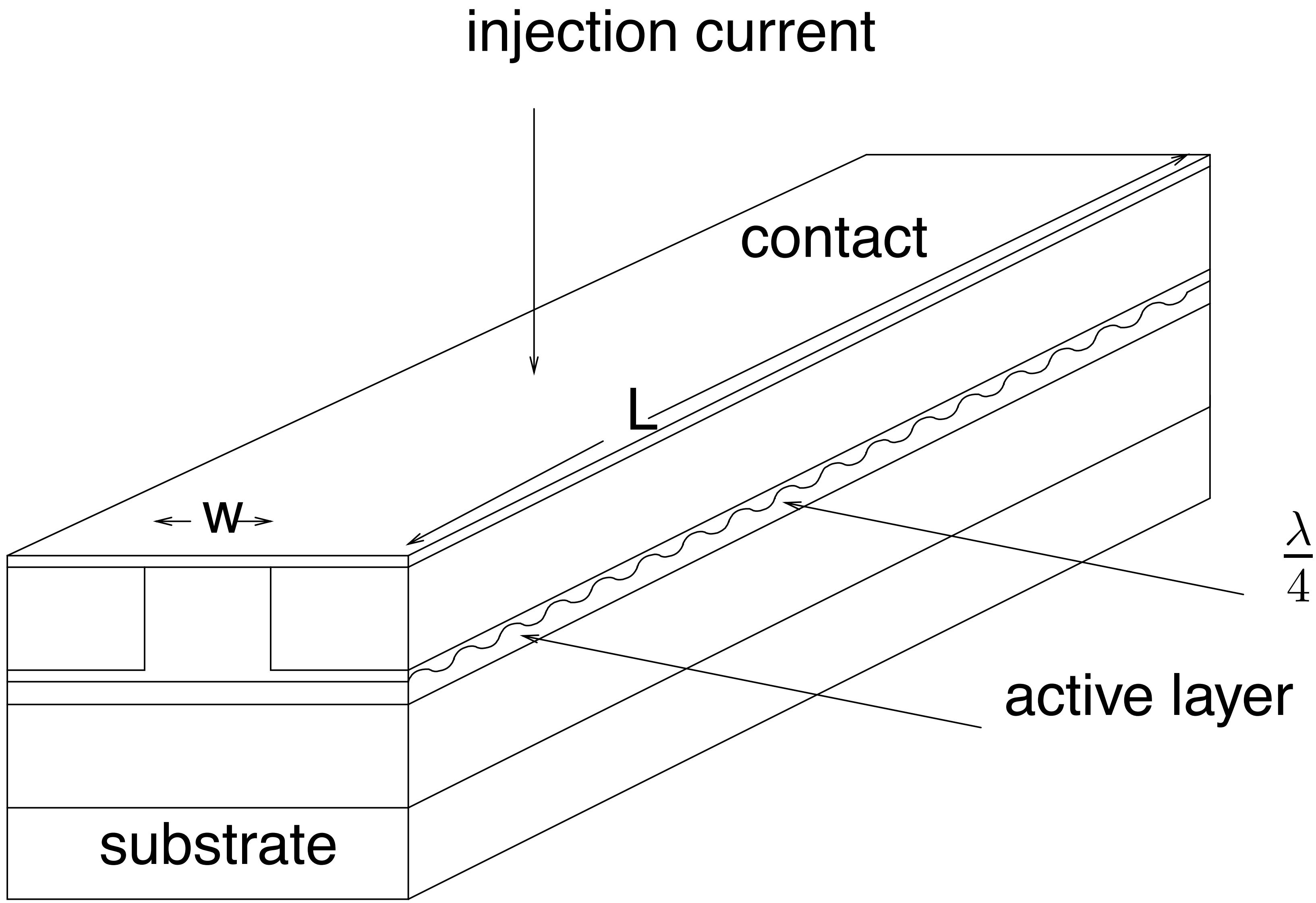


Figure 1: VCSEL (Distributed Feedback Laser)

Distributed Bragg Reflectors (DBR)

Let us assume that the resonator has the form

$$\Omega = \Psi \times [0, L]$$

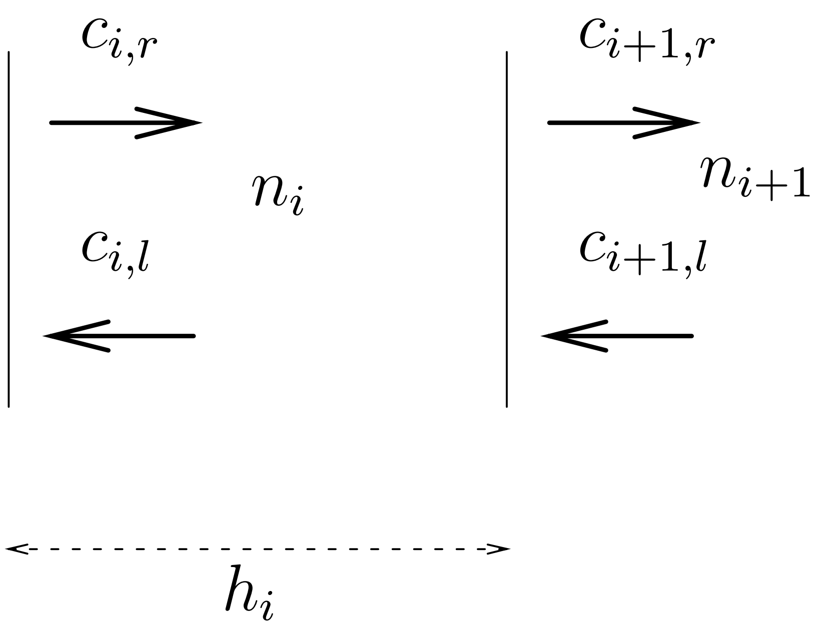
and that $0 = l_0 < l_1 < ... < l_s = L$ Furthermore, let us assume that the resonator has the refraction index n_i (k_i) in the layer $\Psi \times [l_{i-1}, l_i]$. Assume that

$$-E'' - k^2 E = 0.$$

Let us assume the k is constant in the interior of $[l_{i-1}, l_i]$. Then,

$$E(z) = c_{i,r} \exp(-ik_i(z - l_{i-1})) + c_{i,l} \exp(ik_i(z - l_{i-1})) \quad \text{for } z \in [l_{i-1}, l$$

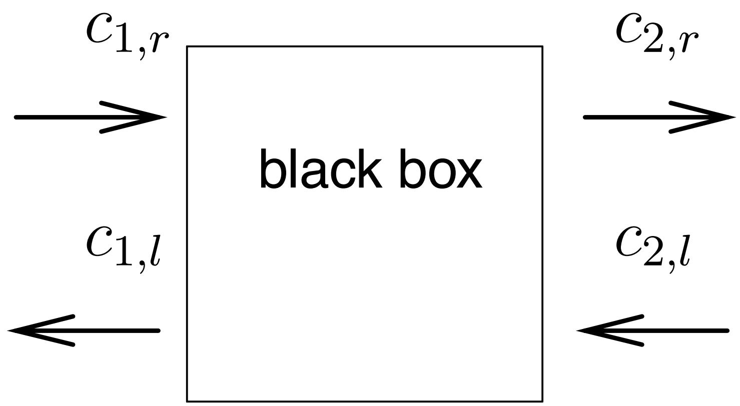
Transmission Matrix of One Layer



$$\begin{pmatrix} c_{i+1,r} \\ c_{i+1,l} \end{pmatrix} = M_i \begin{pmatrix} c_{i,r} \\ c_{i,l} \end{pmatrix}$$

$$M_i = \begin{pmatrix} k_{i+1} + k_i & k_{i+1} - k_i \\ k_{i+1} - k_i & k_{i+1} + k_i \end{pmatrix} \cdot \frac{1}{2k_{i+1}} \begin{pmatrix} \exp(-ik_i h_i) & 0 \\ 0 & \exp(ik_i h_i) \end{pmatrix}.$$

Transmission Matrix and Scattering Matri

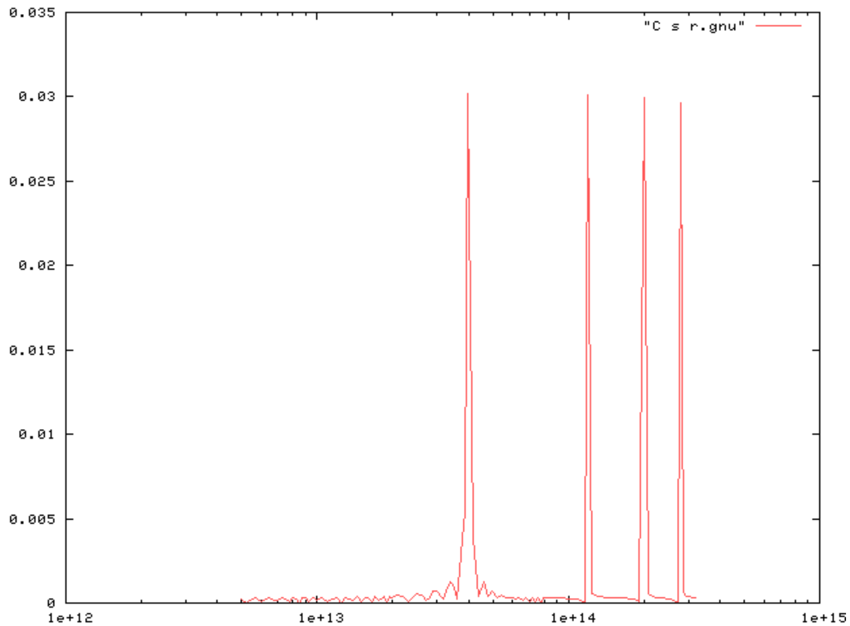


In general one can describe the behavior by a scattering matrix S and a transmission matrix T:

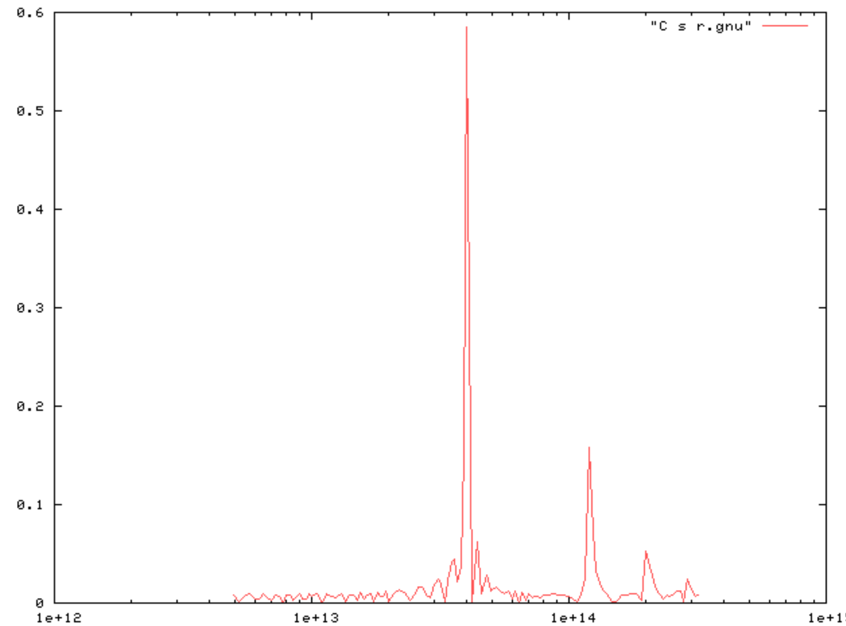
$$\begin{pmatrix} c_{1,r} \\ c_{1,l} \end{pmatrix} = T \begin{pmatrix} c_{2,r} \\ c_{2,l} \end{pmatrix} \qquad \begin{pmatrix} c_{2,r} \\ c_{1,l} \end{pmatrix} = S \begin{pmatrix} c_{1,r} \\ c_{2,l} \end{pmatrix}$$

Reflection Property of DFB

Example 2. *Let us study* 101 *layers with refraction index* $n_0, n_1, n_0, ..., n_0$, $\lambda_0 = 1.6 \cdot 10^{-6}$, $k_0 = \frac{2\pi}{\lambda_0}$, *and* $\omega = \frac{k}{\sqrt{\epsilon_0 \mu_0} n_0}$, *where* $\sqrt{\epsilon_0 \mu_0} = \frac{1}{c}$ *and* $n_0 = 3.277$. *Let us choose* $c_{2,l} = 1$, $c_{1,r} = 0$. *Then,* $c_{1,l}$ *shows the behavior of the construction. A high reflectivity is obtained for* $\omega = \omega_0, 3\omega_0, 5\omega_0, ...$.



Reflection behavior for $n_1 = 3.275$.



Reflection behavior for $n_1 = 3.220$.

Finite Elements of DFB

Let Ω_h be a grid of meshsize h for the domain $\Omega = [0, L]$. Furthermore, let v_p be the nodal basis function with respect to linear elements. Then, define

$$\begin{aligned} v_p^l &= e^{ikz} v_p \\ v_p^r &= e^{-ikz} v_p \\ v_p^m &= \begin{cases} e^{ikz} v_p(z) & \text{for } z \leq p \text{ and} \\ e^{-ikz} v_p(z) & \text{for } z > p. \end{cases} \end{aligned}$$

Now, let us define the FE space

$$V_h^{ref} = \text{span}\{v_p^l, v_p^r, v_p^m \mid p \in \Omega_h\}.$$

This FE space leads to the results as the transfer matrix method. But these basis functions can be extended to 2D and 3D.

Time Discretization

Let us recall the scalar Helmholtz equation (**??**):

$$-\triangle \tilde{E} = -\mu\epsilon \frac{\partial^2}{\partial t^2}\left(\tilde{E}\right).$$

The ansatz

$$\tilde{E}(x,y,z,t) = \exp(i\omega t) E(x,y,z,t)$$

leads to

$$\mu\epsilon \frac{\partial^2 E}{\partial t^2} + i\mu\epsilon\omega \frac{\partial E}{\partial t} = \triangle E + \mu\epsilon\omega^2 E.$$

Since ω^2 is large in comparison to $\mu\epsilon$, we apply the following model:

$$i\mu\epsilon\omega \frac{\partial E}{\partial t} = \triangle E + k^2 E.$$

Time Discretization

Crank-Nicolson discretization of this equation leads to

$$i\mu\epsilon\omega \frac{E^{s+1} - E^s}{\tau} = \frac{1}{2} \left(\triangle E^s + k^2 E^s + \triangle E^{s+1} + k^2 E^{s+1} \right).$$

Let us analyze this equation by Fourier analysis in 2D. Then, for $E^s = a^s \sin(l_x x) \sin(l_y y)$, we obtain

$$a^{s+1} = \frac{\frac{1}{2}(l_x^2 + l_y^2 + k^2) + i\frac{\mu\epsilon\omega}{\tau}}{\frac{1}{2}(l_x^2 + l_y^2 + k^2) - i\frac{\mu\epsilon\omega}{\tau}} a^s$$

This equation implies

$$|a^{s+1}| = |a^s|$$

if $k \in \mathbb{R}$. This means a real k does not lead to a gain or an absorption. An explicit or implicit Euler discretization does not have this property.

Modeling the Wave in a Resonator

Let us assume that $\Omega = \Omega_{2D} \times [0, L]$ is the domain of a laser resonator, where L is the length of the resonator.
Here, let us assume that $E_1, ..., E_M$ are eigenmodes obtained by a Gauss mode analysis or another method.
Thus, $E_i : \Omega \to \mathbb{C}$ are functions, which we normalize as follows

$$\int_{\Omega} |E_i|^2 \, d(x, y, z) = 1.$$

Model Assumption 1

The electrical field E of the total optical wave is approximated by M eigenmodes:

$$E(t,x,y,z) = \sum_{i=1}^{M} \xi_i(t) E_i(x,y,z),$$

where $\xi_i : [t_0, \infty[\to \mathbb{R}$ is the time-dependent coefficient of the i-th mode. Then, the photon density of the mode $\xi_i(t)E_i(x,y,z)$ is

$$n_i(t,x,y,z) \quad = \quad \frac{\epsilon}{2\hbar\omega_i} |\xi_i(t)E_i(x,y,z)|^2 = \frac{\epsilon}{2\hbar\omega_i} \Xi_i(t) |E_i(x,y,z)|^2,$$

where we abbreviate

$$\Xi_i(t) = |\xi_i(t)|^2.$$

Model Assumption 2

The modes are incoherent modes. Here, this means that the total photon density $n(t, x, y, z)$ can be written as

(14) $$n(t, x, y, z) = \sum_{i=1}^{M} n_i(t, x, y, z).$$

Model Assumption 3

The local photon densities $n_i(t,x,y,z)$ and the population inversion density $N(t,x,y,z)$ satisfy the rate equations:

$$\frac{\partial n_i}{\partial t} = N n_i \sigma c - \frac{n_i}{\tau_c} + S, \qquad i = 1, .., M, \tag{15}$$

$$\frac{\partial N}{\partial t} = -\gamma N n \sigma c - \frac{N + N_{\text{tot}}(\gamma - 1)}{\tau_f} + R_{\text{pump}}(N_{\text{tot}} - N). \tag{16}$$

ODE System

$$\frac{\partial \Xi_i}{\partial t} = \Xi_i \int_\Omega N|E_i|^2\, d(x,y,z)\, \sigma c - \frac{\Xi_i}{\tau_c} + \frac{2\hbar\omega_i}{\epsilon} \int_\Omega S\, d(x,y,z), \qquad i =$$

(17)

$$\frac{\partial N}{\partial t} = -\gamma N \sigma c \sum_{i=1}^{M} \frac{\epsilon}{2\hbar\omega_i} \Xi_i |E_i|^2 - \frac{N + N_{\text{tot}}(\gamma - 1)}{\tau_f} + R_{\text{pump}}(N_{\text{tot}} - I$$

(18)

These equations form a solvable system of ordinary differential equations, which describes the time-dependent behavior of M modes. This behavior is mainly influenced by the pump configuration R_{pump}.

Stationary Solution

The solution $(\Xi_i(t))_{i=1,\ldots,M}, N(t,x,y,z)$ can tend to a stationary solution $(\Xi_i^\infty)_{i=1,\ldots,M}, N^\infty(x,y,z)$, which corresponds to the optical wave of a cw-laser. This stationary solution satisfies the equations

$$
\begin{aligned}
0 &= \Xi_i^\infty \int_\Omega N^\infty |E_i|^2 \, d(x,y,z) \, \sigma c - \frac{\Xi_i^\infty}{\tau_c} + \frac{2\hbar\omega_i}{\epsilon} \int_\Omega S \, d(x,y,z), \\
0 &= -\gamma N^\infty \sigma c \sum_{i=1}^{M} \frac{\epsilon}{2\hbar\omega_i} \Xi_i^\infty |E_i|^2 - \frac{N^\infty + N_{\text{tot}}(\gamma - 1)}{\tau_f} + \\
& \quad R_{\text{pump}}(N_{\text{tot}} - N^\infty).
\end{aligned}
$$

Numerical Approximation

For reasons of simplicity, let us assume that

$$\Omega = [-R, R]^2 \times [0, L]$$

is a cuboid. Let Ω_{h_{xy},h_z} be the discretization mesh

$$\Omega_{h_{xy},h_z} = \left\{ \left((i - \frac{1}{2})h_{xy}, (j - \frac{1}{2})h_{xy}, (k - \frac{1}{2})h_z \right) \;\middle|\; i, j = -M_{xy} + 1$$

where $h_{xy} = \frac{R}{M_{xy}}$, $h_z = \frac{L}{M_z}$, and $M_{xy}, M_z \in \mathbb{N}$. To every grid point $p = (x, y, z) \in \Omega_{h_{xy},h_z}$ corresponds a discretization cell

$$c_p = \left] x - \frac{h_{xy}}{2}, x + \frac{h_{xy}}{2} \right[\times \left] y - \frac{h_{xy}}{2}, y + \frac{h_{xy}}{2} \right[\times \left] z - \frac{h_z}{2}, z + \frac{h_z}{2} \right[.$$

Numerical Approximation

Using a finite volume discretization, we approximate $N(t,x,y,z)$, $(x,y,z) \in c_p$, by the constant value $N_p(t)$ for every point $p \in \Omega_{h_{xy},h_z}$.

$$
\begin{aligned}
\frac{\partial \Xi_i}{\partial t} &= \Xi_i \left(\sum_{p \in \Omega_{h_{xy},h_z}} h_{xy}^2 h_z \; N_p |E_i(p)|^2 \right) \sigma c - \frac{\Xi_i}{\tau_c} + \\
& \quad \frac{2\hbar\omega_i}{\epsilon} \int_\Omega S \; d(x,y,z), \qquad\qquad i = 1,..,M, \\
\frac{\partial N_p}{\partial t} &= -\gamma N_p \sigma c \sum_{i=1}^{M} \frac{\epsilon}{2\hbar\omega_i} \Xi_i |E_i(p)|^2 \; \frac{N_p + N_{\text{tot}}(\gamma - 1)}{\tau_f} + \\
& \quad R_{\text{pump}}(p)(N_{\text{tot}} - N_p), \qquad\qquad p \in \Omega_{h_{xy},h_z}.
\end{aligned}
$$

Maxwell's Equations

The solution of Maxwell's equations in 3D is

- $\vec{E}$: the electrical field and
- $\vec{H}$: the magnetic field.

Given are

- μ: magnetic permeability,
- ϵ: electric permittivity,
- $\vec{M}$: equivalent magnetic current density,
- $\vec{J}$: electric current density.

Maxwell's equations are:

$$\begin{aligned}
\frac{\partial \vec{H}}{\partial t} &= -\frac{1}{\mu}\nabla \times \vec{E} - \frac{1}{\mu}\vec{M} \\
\frac{\partial \vec{E}}{\partial t} &= \frac{1}{\epsilon}\nabla \times \vec{H} - \frac{1}{\epsilon}\vec{J}
\end{aligned}$$

Finite Difference Time Domain Discretizati

Let τ be a time step.

Time approximation:

- $\vec{E}|^{n+\frac{1}{2}}$: approximation at time point $(n+\frac{1}{2})\tau$.
- $\vec{H}|^{n}$: approximation at time point $n\tau$.

Furthermore, let us use the following abbreviation:

$$\begin{aligned} \vec{H}|^{n+\frac{1}{2}} &:= \frac{1}{2}\left(\vec{H}|^{n+1} + \vec{H}|^{n}\right), \\ \vec{E}|^{n} &:= \frac{1}{2}\left(\vec{E}|^{n+\frac{1}{2}} + \vec{E}|^{n-\frac{1}{2}}\right). \end{aligned}$$

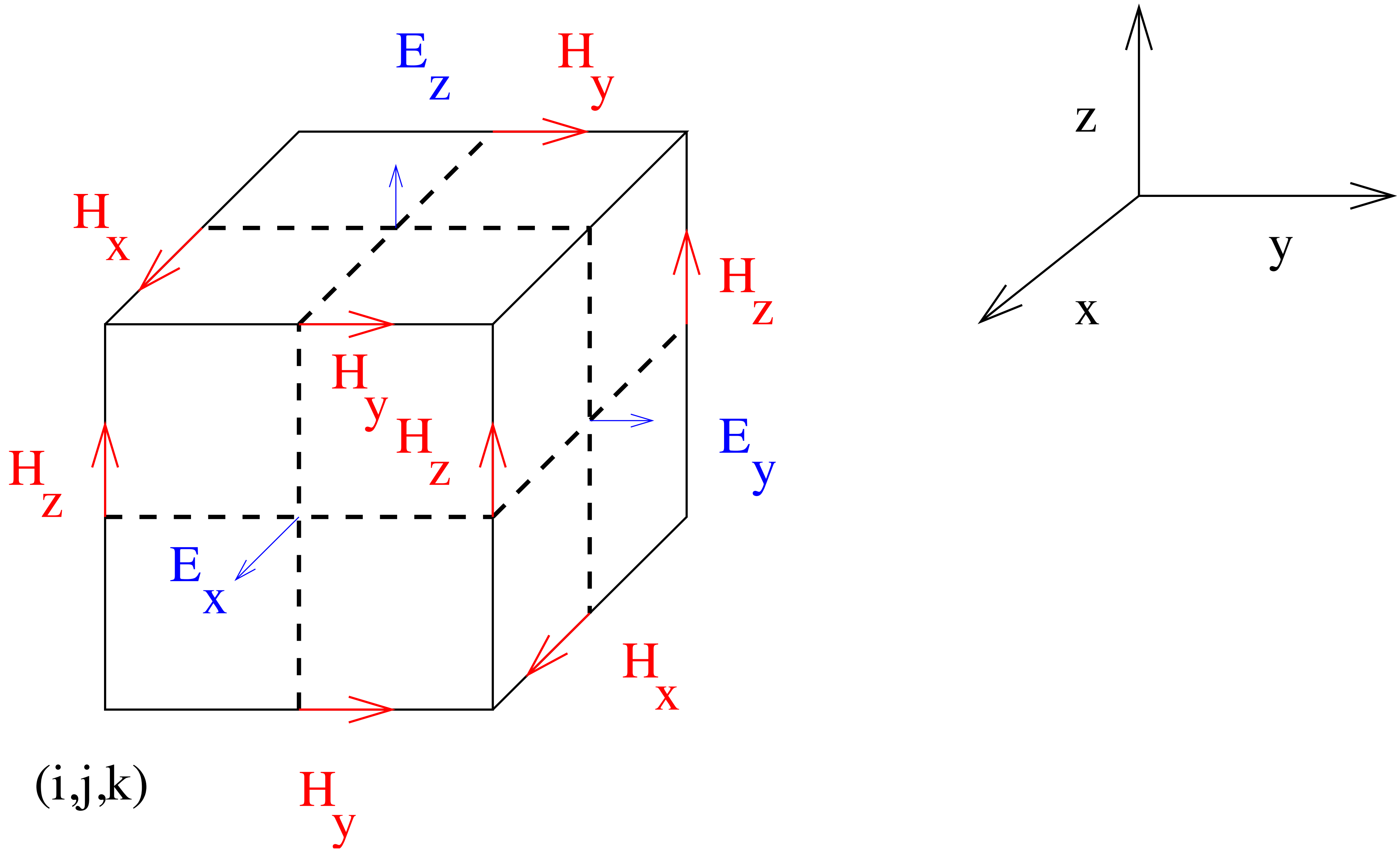
FDTD

Let h be a mesh size.

<u>Space approximation:</u>

- $E_x|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}}$: at point $(ih, (j+\frac{1}{2})h, (k+\frac{1}{2})h)$ (yz-face) .
- $E_y|^{n+\frac{1}{2}}_{i+\frac{1}{2},j,k+\frac{1}{2}}$: at point $((i+\frac{1}{2})h, jh, (k+\frac{1}{2})h)$ (xz-face).
- $E_z|^{n+\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2},k}$: at point $((i+\frac{1}{2})h, (j+\frac{1}{2})h, kh)$ (xy-face).
- $H_x|^{n}_{i+\frac{1}{2},j,k}$: at point $((i+\frac{1}{2})h, jh, kh)$ (x-edge).
- $H_y|^{n}_{i,j+\frac{1}{2},k}$: at point $(ih, (j+\frac{1}{2})h, kh)$.
- $H_z|^{n}_{i,j,k+\frac{1}{2}}$: at point $(ih, jh, (k+\frac{1}{2})h)$.

FDTD



Staggered Grid Discretization

Now, the Maxwell equation

$$\frac{\partial E_x}{\partial t} = -\frac{1}{\epsilon}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} + J_x\right)$$

is discretized as follows:

$$\frac{E_x|^{n+\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}} - E_x|^{n-\frac{1}{2}}_{i,j+\frac{1}{2},k+\frac{1}{2}}}{\tau} =$$

$$\frac{1}{\epsilon_{i,j+\frac{1}{2},k+\frac{1}{2}}} \left(\frac{H_z|^n_{i,j+1,k+\frac{1}{2}} - H_z|^n_{i,j,k+\frac{1}{2}}}{h} - \frac{H_y|^n_{i,j+\frac{1}{2},k+1} - H_y|^n_{i,j+\frac{1}{2},k}}{h} - J_x|^n_{i,j+\frac{1}{2},k+\frac{1}{2}}\right)$$

The other Maxwell's equations are discretized analogously.

Staggered Grid Discretization

Let ∂_τ^1 the symmetric difference operator applied to the time coordinate:

$$\partial_h^1 Q(t) := \frac{Q(t+\tau/2) - Q(t-\tau/2)}{\tau}$$

Furthermore, let $\nabla_h \times$ the discrete curl operator on a staggered grid. Then the FDTD discretization can be described as follows:

$$\begin{aligned}
\partial_\tau^1 \vec{H}_{h,\tau} &= -\frac{1}{\mu}\nabla_h \times \vec{E}_{h,\tau} - \frac{1}{\mu}\vec{M}_{h,\tau} \quad \text{at time points } n+\tfrac{1}{2}, \\
\partial_\tau^1 \vec{E}_{h,\tau} &= \frac{1}{\epsilon}\nabla_h \times \vec{H}_{h,\tau} - \frac{1}{\epsilon}\vec{J}_{h,\tau} \quad \text{at time points } n.
\end{aligned}$$

Here, $\vec{H}_{h,\tau}$ and $\vec{E}_{h,\tau}$ are the vectors on a staggered grid.

Losses

$\vec{J}$ has to be composed as follows:

$$\vec{J} = \vec{J}_{source} + \sigma\vec{E},$$

where σ is the electric conductivity.
$\vec{E}$ is approximated by

$$\vec{E}\Big|^{n} = \frac{1}{2}\left(\vec{E}\Big|^{n+\frac{1}{2}} + \vec{E}\Big|^{n-\frac{1}{2}}\right).$$

Boundary Conditions

Reflecting boundary conditions can be modeled by pure Dirichlet boundary conditions.
Non-reflecting boundary conditions can be discretized by the Perfect Matched Layer (PML) method. These are not Neumann boundary conditions!

Stability of FDTD

Let us consider the FDTD discretization in the short form for $\vec{J}_{h,\tau} = 0$ and $\vec{M}_{h,\tau} = 0$ and $\mu = 1$ and $\epsilon = 1$:

$$\begin{aligned} \partial_\tau^1 \vec{H}_{h,\tau} &= -\nabla_h \times \vec{E}_{h,\tau} \quad \text{at time points } n + \tfrac{1}{2}, \\ \partial_\tau^1 \vec{E}_{h,\tau} &= \nabla_h \times \vec{H}_{h,\tau} \quad \text{at time points } n. \end{aligned}$$

Now, the abbreviation

$$\vec{V}_{h,\tau} = \vec{H}_{h,\tau} + j\vec{E}_{h,\tau}$$

leads to

$$\partial_\tau^1 \vec{V}_{h,\tau} = j\nabla_h \times \vec{V}_{h,\tau}$$

Stability of FDTD

Definition 2. *The FDTD method is stable, if the solution $\vec{H}_{h,\tau}, \vec{E}_{h,\tau}$ is bounded for $t \to \infty$.*

Let us analyze

$$\partial_\tau^1 \vec{V}_{h,\tau} = j\nabla_h \times \vec{V}_{h,\tau}.$$

To this end, it is enough to analyze the behavior of the solutions with periodic initial condition:

$$\vec{V}_{h,\tau}(0, x, y, z) = \vec{V}_0 e^{j(-k_x x - k_y y - k_z z)}. \tag{19}$$

The FDTD method is stable, if $\vec{V}_{h,\tau}$ has the form

$$\vec{V}_{h,\tau}(t, x, y, z) = \vec{V}_0 e^{j(\omega t - k_x x - k_y y - k_z z)}$$

Stability of FDTD

The abbreviation $\vec{V}_0 = (V_x, V_y, V_z)^T$ leads to

$$
\begin{aligned}
\nabla_h \times \vec{V}_{h,\tau} &= \text{det} \begin{pmatrix} e_x & \delta^1_{h_x,x} & V_x \\ e_y & \delta^1_{h_y,y} & V_y \\ e_z & \delta^1_{h_z,z} & V_z \end{pmatrix} e^{j(\omega t - k_x x - k_y y - k_z z)} \\
&= \text{det} \begin{pmatrix} e_x & \frac{1}{h_x}\sin(\frac{k_x h_x}{2}) & V_x \\ e_y & \frac{1}{h_y}\sin(\frac{k_y h_y}{2}) & V_y \\ e_z & \frac{1}{h_z}\sin(\frac{k_z h_z}{2}) & V_z \end{pmatrix} e^{j(\omega t - k_x x - k_y y - k_z z)} \\
&= -j\frac{1}{\tau}\sin(\frac{\omega\tau}{2}) \begin{pmatrix} V_x \\ V_y \\ V_z \end{pmatrix} e^{j(\omega t - k_x x - k_y y - k_z z)}
\end{aligned}
$$

Stability of FDTD

The above equation system has a unique solution if and only if

$$
\begin{aligned}
0 &= \det \begin{pmatrix} j\frac{1}{\tau}\sin(\frac{\omega\tau}{2}) & \frac{1}{h_z}\sin(\frac{k_z h_z}{2}) & -\frac{1}{h_y}\sin(\frac{k_y h_y}{2}) \\ \frac{1}{h_z}\sin(\frac{k_z h_z}{2}) & j\frac{1}{\tau}\sin(\frac{\omega\tau}{2}) & -\frac{1}{h_x}\sin(\frac{k_x h_x}{2}) \\ -\frac{1}{h_y}\sin(\frac{k_y h_y}{2}) & +\frac{1}{h_x}\sin(\frac{k_x h_x}{2}) & j\frac{1}{\tau}\sin(\frac{\omega\tau}{2}) \end{pmatrix} \\
&= \left(\left(\frac{1}{h_x}\sin(\frac{k_x h_x}{2})\right)^2 + \left(\frac{1}{h_y}\sin(\frac{k_y h_y}{2})\right)^2 + \left(\frac{1}{h_z}\sin(\frac{k_z h_z}{2})\right)^2 \right. \\
&\quad \left. - \left(\frac{1}{\tau}\sin(\frac{\omega\tau}{2})\right)^2 \right) j\frac{1}{\tau}\sin(\frac{\omega\tau}{2})
\end{aligned}
$$

. This is equivalent to the *stability equation:*

$$
\left(\frac{1}{h_x}\sin(\frac{k_x h_x}{2})\right)^2 + \left(\frac{1}{h_y}\sin(\frac{k_y h_y}{2})\right)^2 + \left(\frac{1}{h_z}\sin(\frac{k_z h_z}{2})\right)^2 = \left(\frac{1}{\tau}\sin(\frac{\omega\tau}{2})\right)^2
$$

Stability of FDTD

The *stability equation* has a solution ω for every k_x, k_y, k_z, if

$$\tau\sqrt{\frac{1}{h_x^2}+\frac{1}{h_y^2}+\frac{1}{h_z^2}} < 1.$$

A renormalization of this stability condition shows

$$\tau < c^{-1}\left(\frac{1}{h_x^2}+\frac{1}{h_y^2}+\frac{1}{h_z^2}\right)^{-\frac{1}{2}}.$$

where c is the velocity of the wave.