# Simulation und wissenschaftliches Rechnen 2

Übung

Sommersemester 2013 - Rüde

# Contents

# 1 Recapitulation

$$-u''(x) = f(x) \qquad \text{for} 0 \leq x \leq 1 \tag{1.1}$$
$$u(0) = u(1) = 0 \tag{1.2}$$

spacial discretization: finite difference approximation:

$$u_i''(x) \approx \frac{u_i(x-h) - 2u_i(x) + u_i(x+h)}{h^2} \tag{1.3}$$

stencil notation:

$$\frac{1}{h^2}\begin{bmatrix} -1 & +2 & -1 \end{bmatrix} \tag{1.4}$$

this results in the following LSE (linear system of equations) for $n = 6$:

$$\underbrace{\frac{1}{h^2}\begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}}_{A} \cdot \underbrace{\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}}_{\vec{u},\ \text{innere Knoten}} = \underbrace{\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}}_{\vec{f}} + \underbrace{\begin{bmatrix} h^2u(0) \\ 0 \\ 0 \\ 0 \\ h^2u(6) \end{bmatrix}}_{\text{Dirichlet BCs}} \tag{1.5}$$

can be solved by iterative methods: $\rightsquigarrow$ compute in each iteration an approximation $\tilde{u}_i$ of $u_i$ .

Equation for each point:

$$\frac{-\tilde{u}_i(x-h) + 2\tilde{u}_i(x) - \tilde{u}_i(x+h)}{h^2} = f_i(x) \tag{1.6}$$
$$\rightarrow -\tilde{u}_i(x-h) + 2\tilde{u}_i(x) - \tilde{u}_i(x+h) = h^2 f_i(x)$$

### Jacobi's method

$$\tilde{u}_i^{k+1} = \frac{1}{2}(\tilde{u}_{i-1}^k + \tilde{u}_{i+1}^k + h^2 f_i) \qquad \text{for } k\text{-th iteration} \tag{1.7}$$

### Gauss-Seidel method

$$\tilde{u}_i^{k+1} = \frac{1}{2}(\tilde{u}_{i-1}^{k+1} + \tilde{u}_{i+1}^k + h^2 f_i) \tag{1.8}$$

## 1.1 FD- Discretisation of Laplace Operator

$$\Delta u = \frac{\delta^2 u}{\delta x^2} + \frac{\delta^2 u}{\delta y^2} \tag{1.9}$$

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &\approx \frac{u(x+h,y) - 2u(x,y) + u(x-h,y)}{h^2} \\ \frac{\partial^2 u}{\partial y^2} &\approx \frac{u(x,y+h) - 2u(x,y) + u(x,y-h)}{h^2} \end{aligned}$$

stencil notation:

$$\frac{1}{h^2}\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{1.10}$$

## 1.2 Grid Layout

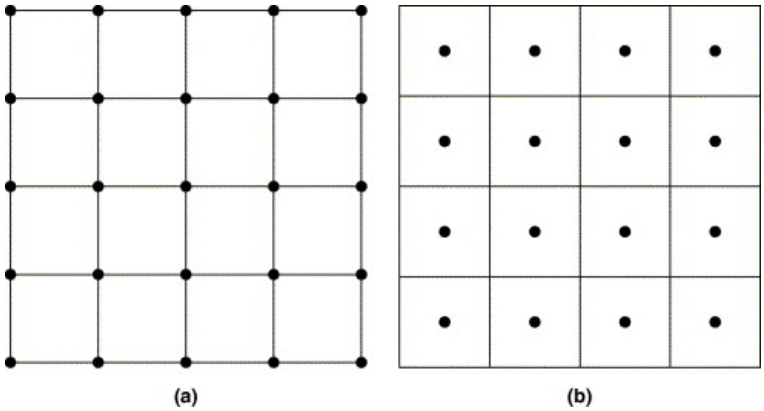


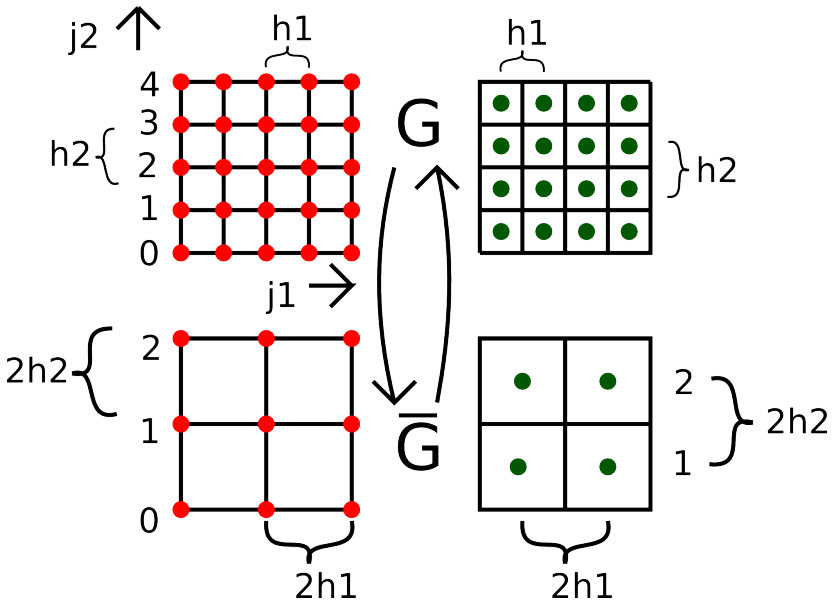

Figure 1.1: vertex centered (a) and cell-centered (b) grid layout

Vertex-centered grid:

$$G = \{x \in \overline{\Omega} : x = jh; j = (j_1, j_2); j_2 = 0, 1, 2, \ldots, n_2; h = (h_1, h_2); h_2 = \frac{1}{n_2}\}$$

Cell-centered grid:

$$G = \{x \in \Omega : x = x_j = (j - s)h; j = (j_1, j_2); s = (\frac{1}{2}, \frac{1}{2}); h = (h_1, h_2); h_2 = \frac{1}{n_2}; j_2 = 1, 2, 3, \ldots, n_2\}$$




## 1.3 Coarsening

## 1.4 Multigrid Stencil

**Restriction** Transports residual of fine grid to coarser grid. Full weighting restriction:

$$I_l^{l-1} = \frac{1}{16}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix} \tag{1.11}$$

**Prolongation** Transports obtained correction on coarse grid to fine grid. Linear interpolation:

$$I_{l-1}^{l} = \frac{1}{4}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix} \tag{1.12}$$

**Boundary Conditions** *Dirichlet:*

$$u|_{\delta\Omega} = \text{ given value / function} \tag{1.13}$$

1. set all boundary points, initialize grid (precondition)
2. perform red-black GS: iterate over all iteration points, *not* boundary points

*Neumann:*

$$\frac{\partial u}{\partial n^s}|_{\partial\Omega} = 0 \tag{1.14}$$

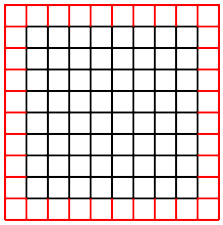


Figure 1.2: vertex-centerd grid with ghost layer

1. Add ghost-layer
2. initialize grid
3. iterate over *all* points of domain (but *not* ghost)
4. loop over all Neumann-boundaries (use central differences)

$$\frac{\partial u}{\partial n^s} = 0 \qquad \frac{u(0,g) - u(1,g)}{h} = 0 \qquad \rightarrow u(0,g) = u(1,g)$$

   $\rightsquigarrow$ better in cell-centered

# 2 Multigrid

Multigrid (MG) consists of the following two basic ideas:

1. the residual equation
2. the smoothing property of relaxation schemes

## 2.1 The residual equation

Let

$$A\vec{u} = \vec{f} \tag{2.1}$$

denote an LSE (linear system of equations) and

$$\vec{e} = \vec{u} - \vec{v} \tag{2.2}$$

denote the (algebraic) error of the approximation $\vec{v}$

Since the error is just as inaccessible as the exact solution itself (if we knew the error we knew the solution) we use the residuum:

$$\vec{r} = \vec{f} - A\vec{v} \tag{2.3}$$

(If $\vec{v}$ was exact solution: $u = A\vec{u} = A\vec{v} = \vec{f} \Rightarrow \vec{r} = 0$). Note: $\vec{r}$ is small in norm doesn't imply $\vec{e}$ is small in norm.

Using 2.1, 2.2 and 2.3 gives the so called residual equation:

$$A\vec{e} = \vec{r} \tag{2.4}$$

## 2.2 Smoothing properties

### 2.2.1 Error convergence

**Jacobi method** one row from equation system/matrix

$$v_i^{(1)} = \frac{1}{2}( \underbrace{v_{i-1}^{(0)}}_{leftneighbour} + \underbrace{v_{i+1}^{(0)}}_{rightneighbour} + h^2 f_i) \qquad 1 \leq i \leq n-1; n = \frac{1}{n}$$

$$\Rightarrow \frac{1}{h^2}[-1 \quad 2 \quad -1] \cdot \begin{pmatrix} v_{i-1} \\ v_i \\ v_{i+1} \end{pmatrix} = f_i$$

split : $A = D - L - U$

$$\vec{v}^{(1)} = \underbrace{D^{-1}(L+U)}_{R_J}\vec{v}^{(0)} + D^{-1}\vec{f}$$

general matrix form:

$$\vec{v}^{(m+1)} = R_J\vec{v}^{(m)} + \vec{g} \tag{2.5}$$

### Damped Jacobi method

$$\vec{v}^{(m+1)} = \underbrace{[(1-\omega)I + \omega R_J]}_{R_\omega}\vec{v}^{(m)} + \underbrace{\omega D^{-1}f}_{g} \tag{2.6}$$

### General formulation

$$\vec{v}^{(m+1)} = R\vec{v}^{(m)} + \vec{g} \qquad \text{approximation} \tag{2.7}$$

$$\vec{u} = R\vec{u} + \vec{g} \qquad \text{exact solution} \tag{2.8}$$

(2.7 - 2.8):

$$\vec{e}^{(m+1)} = R\vec{e}^{(m)}$$

$$\vec{e}^{(m)} = R^m\vec{e}^{(0)}$$

$$||\vec{e}^{(m)}|| \leq ||R^m|| \cdot ||\vec{e}^{(0)}||$$

It is known that $\lim_{m\to\infty} R^m = 0$ if and only if $\rho(R) < 1$ ($R^m$: convergence factor; $\rho(R)$ : spectral radius, asymptotic convergence factor; $\rho(R) = \max|\lambda(R)|$).

### 2.2.2 Example problem

For the following study of linear iterations we will use the homoeneous linear system of equations:

$$A\vec{u} = 0$$

and arbitrary initial guesses to start the relaxation scheme. $\Rightarrow$ Solution is known ($u = 0$) and the error is simply $e = -v$.

Problem formulation (1d):

$$-u''(x) = 0$$

$$u(0) = u_0 = u(1) = 0$$

Obtain insight into smoothing properties by applying various iterations to this system of equations with initial guesses consisting of the vectors (or Fourier modes):

$$v_i = \sin(\frac{ik\pi}{n}), \qquad 0 \leq i \leq n, 1 \leq k \leq n-1 \tag{2.9}$$

k is called wavenumber (frequency) and gives the number of half sine waves on the interval.

### Experimental results

Initial guesses of wavenumbers $k = 1, 3, 6$. We first apply the damped Jacobi method with $\omega = \frac{2}{3}$ to the problem. We use $n = 64$ and $m = 100$ iterations.

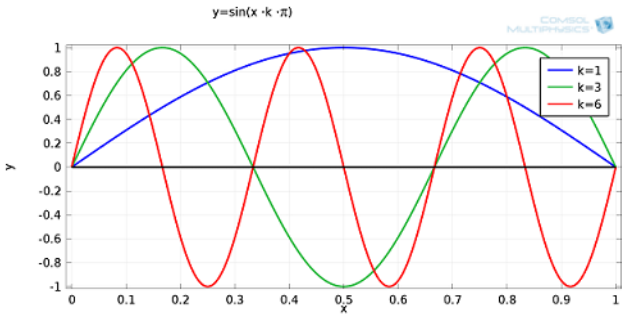



Figure 2.1: Initial guess of wavenumbers

Plot the maximum norm of the error vs. iterations. Observation: the higher $k$, the faster error reduction.

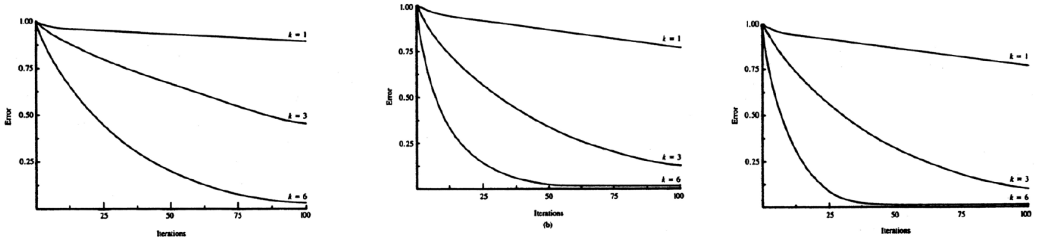


Figure 2.2: Maximum norm of the error of weighted Jacobi ($\omega = \frac{2}{3}$), Gauss-Seidel and Red-Black Gauss-Seidel

Logarithm of the maximum norm $\rightarrow$ geometric decrease $\Rightarrow ||\vec{e}^{(m)}||_\infty = c_k^m ||\vec{e}^{(0)}||$

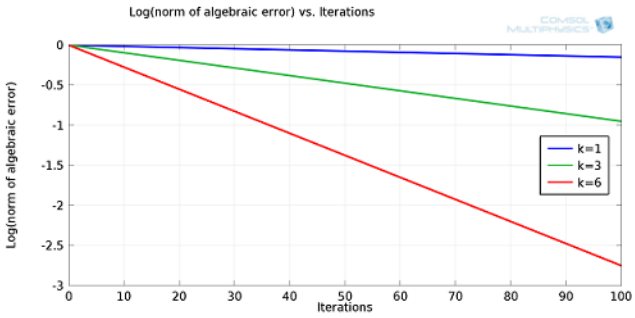



Figure 2.3: Weighted Jacobi with $\omega = \frac{2}{3}$, log(error) is plotted

More realistic, mixed-mode initial guess:

$$v_1 = \frac{1}{3}[\sin(\frac{i\pi}{n}) + \sin(\frac{6i\pi}{n}) + \sin(\frac{32i\pi}{n})]$$

Observation: very quick convergence as long as error has high frequency modes. Performance degradation due to slow elemination of low-frequency components.

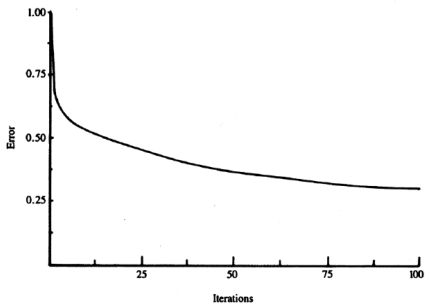



Figure 2.4: Maximum norm of error vs. iterations

### Analytical approach

Compute spectral radius of $R_\omega$ of damped Jacobi method

$$R_\omega = (1-\omega)I + \omega R_J = I - \frac{\omega}{2}A \tag{2.10}$$

Written in this form it follows that eigenvalues $\lambda$ of $R_\omega$ and of $A$ are related by $\lambda R_\omega = 1 - \frac{\omega}{2}\lambda A$.

Eigenvalues of $A$ (known): $\lambda_k(A) = 4\sin^2(\frac{k\pi}{2n}), 1 \le k \le n-1.$
Eigenvectors of $A$: $w_{k,i}(A) = \sin(\frac{ik\pi}{n}, 1 \le k \le n-1, 0 \le n \le 1$

$\Rightarrow$ Eigenvalues of $R_\omega$: $\lambda_k(R_\omega) = 1 - 2\omega\sin^2(\frac{k\pi}{2n})$. Eigenvectors of $R_\omega$: $w_{i,k}(A)$.

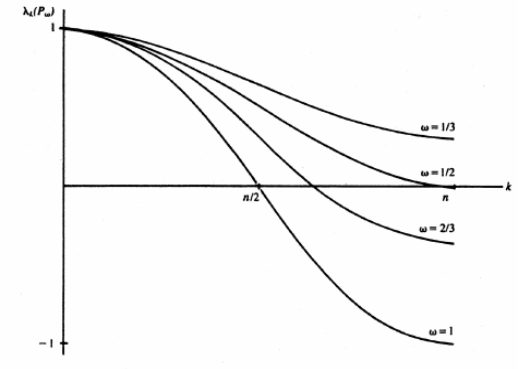



Figure 2.5: Eigenvalues of $R_\omega$, plotted as if $k$ were a continous variable on the interval $0 \le k \le n-1$

Observation $\lambda_1$ associated with smoothest mode always close to 1. Standard Jacobi ($\omega = 1$) efficiently only damps medium-frequency errors.

Goal: Find the value $\omega$ that makes $|\lambda_k(R_\omega)|$ as small as possible for all $1 \leq k \leq n-1$.

Notice that for all $\omega$ satisfying $0 < \omega \leq 1$

$$\lambda_1 = 1 - 2\omega \sin^2(\frac{\pi}{2n}) \underbrace{=}_{h=\frac{1}{n}} 1 - 2\omega \sin^2(\frac{\pi h}{2}) \approx 1 - \frac{\omega \pi^2 h^2}{2}$$

$\Rightarrow \lambda_1$ will always be close to 1. Attempts to improve the accuracy of the solution (by decreasing h) will worsen convergence of smooth error components. $\Rightarrow$ no value of $\omega$ will efficiently reduce smooth error components.

Best damping of oscillatory components ($\frac{n}{2} \leq k \leq n-1$):

$$\lambda_{\frac{n}{2}}(R_\omega) = -\lambda_n(R_\omega) \Rightarrow \omega = \frac{2}{3}$$

$\Rightarrow |\lambda_k| < \frac{1}{3}$; oscillatory components are reduced by a factor 3 (smoothing factor).

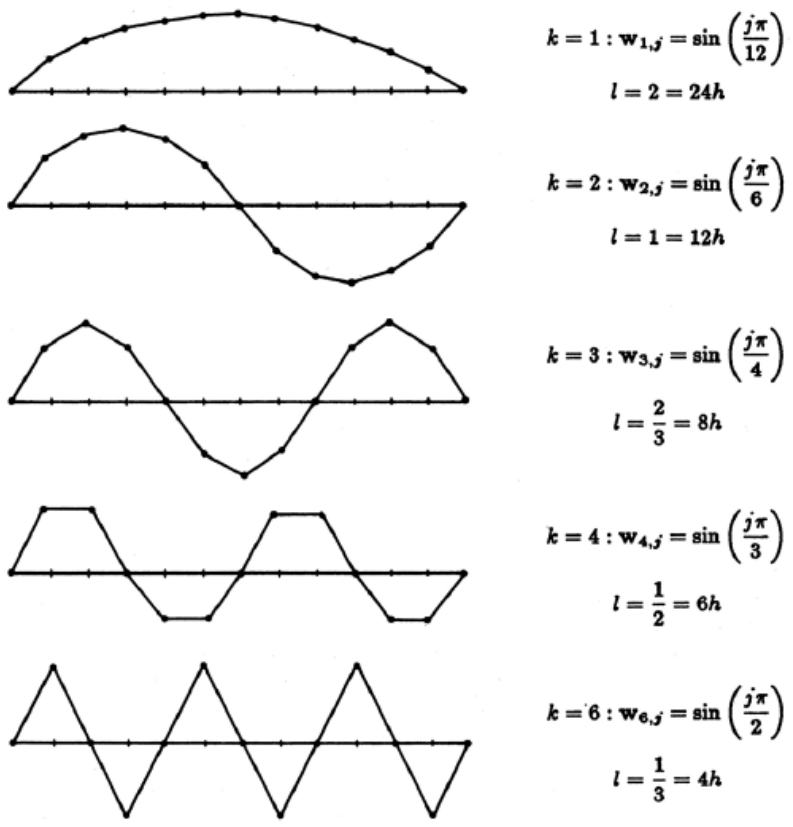



Figure 2.6: Fourier modes of $A$ (and $R_\omega$) on a grid with $n = 12$.

Terminology: Low-frequency / smooth modes: $1 \leq k < \frac{n}{2}$, high-frequency /rough/ oscillatory modes: $\frac{n}{2} \leq k \leq n-1$.

Numerical experiments: Test scenary with $n = 64$ and single Fourier modes $w_k$ with $1 \leq k \leq n-1$ as initial guesses. Damped Jacobi with a) $\omega = 1$ and b) $\omega = \frac{2}{3}$. Number of iterations to reduce initial error by factor 100 for each $w_k$.

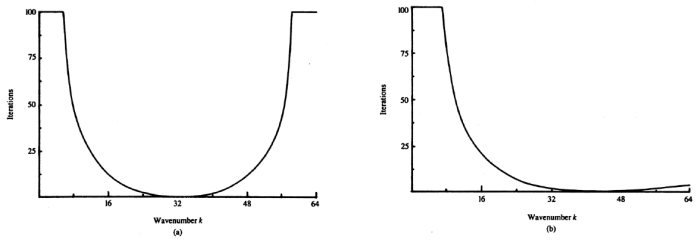



Figure 2.7: a) $\omega = 1$ and b) $\omega = \frac{2}{3}$

Observation: a) Modes with $k$ near $\frac{n}{2}$ damped efficiently, b) Modes with $\frac{n}{2} \leq k \leq n-1$ damped efficiently.

Actual approximate solution after one and 100 iterations.

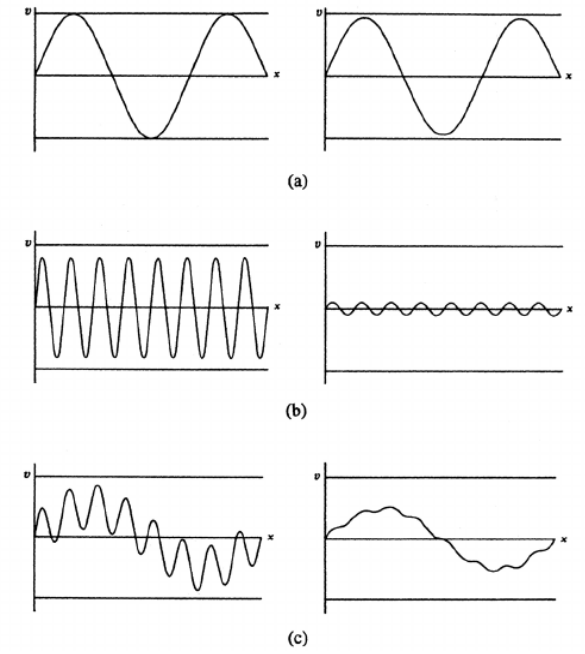



Figure 2.8: Weighted Jacobi with $\omega = \frac{2}{3}$ applied to model problem with initial guess a)$w_3$, b)$w_{16}$ and c)$(w_3 + w_{16})/2$

a) Low frequency mode $w_3 \to e(= -\omega)$ hardly reduced.

b) High frequency mode $w_{16} \to e$ strongly reduced.

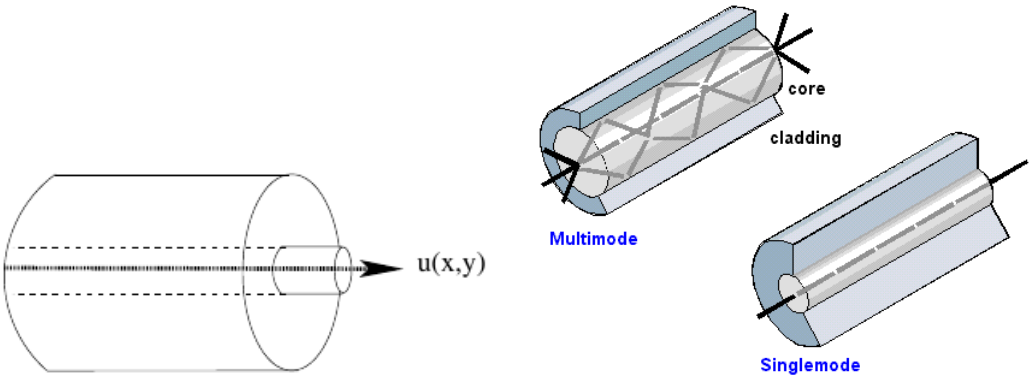
c) Mixed-mode of $w_3$ and $w_{16} \to$ only $e$ of $w_16$ reduced.

# 3 Optical Waveguide

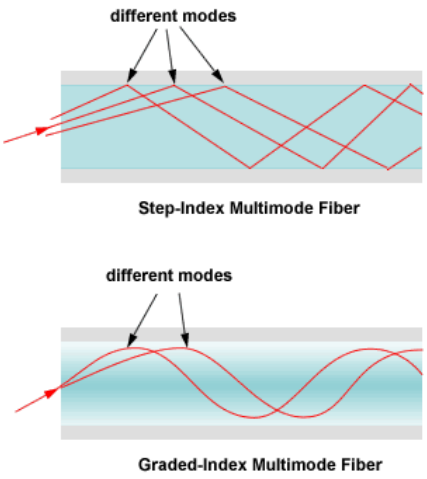
## 3.1 Background

A optical waveguide is a physical structure that guides electromagnetic waves in the optical spectrum. It is used for transmitting light over long distances (e.g. telecommunication systems) and maintaining high optical intensities over appreciable length. It is a spacially inhomogeneus structure for guiding light, i.e. restricting the spacial region in which light can propagate inside the waveguide.

Usually a waveguide contains a region (core) of increased refractive index compared to the surrounding medium (cladding).




One can distinguish two kinds of fibres: step-index-fibres and gradient-index-fibres.



Most waveguides exhibit two-dimensional guidance (in $x-y-$plane), thus restricting the extension of the guided light in 2 dimensions in such a way that propagation is permitted essentially only in 1 dimension ($z$-direction).

## 3.2 Physics

The behaviour of light in the waveguide can be explained by total reflection and ray optics. [1] However, ray optics are invalid when interference occurs, as in small waveguide structures $\Rightarrow$ wave

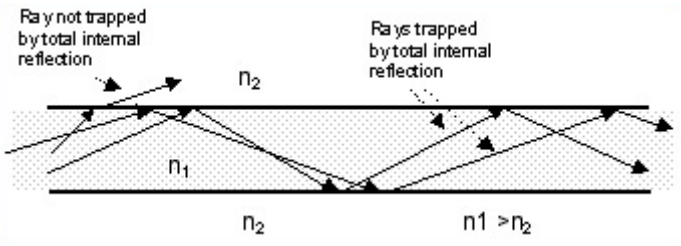



Figure 3.1: Rays can be trapped in a waveguide through total internal reflection.

description of light is required.

By Maxwell's equations and approximate assumptions one obtains the Helmholtz equation:

- Faraday's law: $\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$
- Maxwell-Ampere's law: $\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t}$

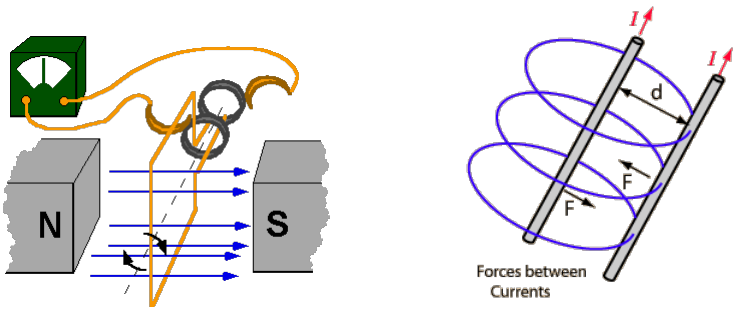



Figure 3.2: Experiment for Farady's law (left) and Maxwell-Ampere's law

- Gauss's law: $\nabla \cdot \vec{D} = \rho$
- Gauss's law magnetic: $\nabla \cdot \vec{B} = \vec{0}$
- Continuity equation: $\nabla \cdot J = -\frac{\partial \rho}{\partial t}$

[1] Picture from `http://osa.magnet.fsu.edu/tutorials/snell.html`

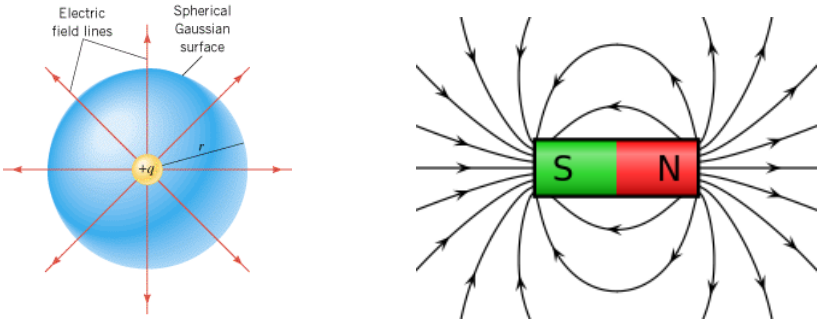



Figure 3.3: Gauss's law and Gauss's law magnetic

- $$\vec{D} = \underbrace{\varepsilon}_{permittility}\vec{E} \qquad \vec{B} = \underbrace{\mu}_{permeability}\vec{H} \qquad \vec{J} = \underbrace{\sigma}_{conductivity}\vec{E}$$

Assumptions: $\mu$ is approximatly constant, $\rho = J = 0$ (no free charges, no convection currents).

$$\nabla \times \nabla \times \vec{E} = \nabla \times \left(-\frac{\partial B}{\partial t}\right) \overset{v=const.}{\underset{B=\mu H}{=}} -\mu\nabla \times \frac{\partial H}{\partial t} = -\mu\frac{\partial(\nabla \times H)}{\partial t} \overset{J=0!}{=} -\mu\frac{\partial^2 \vec{D}}{\partial t^2}$$

$$\Rightarrow \nabla \times \nabla \times \vec{E} = -\mu\frac{\partial^2 \varepsilon E}{\partial t} \qquad \text{Vector Helmholtz equation} \tag{3.1}$$

As $\nabla \times \nabla \times \vec{E} = \nabla(\nabla \cdot \vec{E}) - \Delta\vec{E}$:

$$\nabla(\nabla \cdot \vec{E}) - \Delta\vec{E} = -\mu\frac{\partial^2 \varepsilon E}{\partial t^2}$$

As for transverse electric waves $\varepsilon$ is constant in time: $\nabla(\nabla \cdot \vec{E}) = 0$

$$-\Delta\vec{E} = -\mu\varepsilon\frac{\partial^2 E}{\partial t^2} \qquad \text{scalar Helmholtz equation} \tag{3.2}$$

It is common to consider the field distribution for a given optical frequency and polarization in a plane perpendicular to the propagation direction. Of special interes are those distributions that do not change during propagation apart from a common phase value. Such distributions are associated with so-called waveguide (eigen)modes.

Derivation of eigenvalue problem:

$$\begin{aligned} -\mu\varepsilon\frac{\partial^2 \vec{E}}{\partial t^2} = -\Delta\vec{\tilde{E}}, \quad \tilde{E} = \tilde{E}(x,y,z) \cdot e^{i\omega t} \\ \Leftrightarrow \mu\varepsilon\omega^2\vec{E}(x,y,z)e^{i\omega t} = -\Delta\vec{E}e^{i\omega t} \\ \Leftrightarrow -\Delta\vec{E} - \underbrace{\mu\varepsilon\omega^2}_{k^2 = k_f^2 n^2(x,y)}\vec{E} = \vec{0} \end{aligned}$$

Reminder: $k = \frac{2\pi}{\lambda}$ (wavenumber), $\omega = \frac{2\pi}{T}$ (angular frequency), $E = u(x,y)e^{i(k_f z)}$

$$-\Delta\vec{E} - \underbrace{\mu\varepsilon\omega^2}_{k^2=k_f^2 n^2(x,y)}\vec{E} = \vec{0}$$

$$\underbrace{-\Delta xyu(x,y)e^{i(k_f z)}}_{\text{Laplace for x and y dir.}} - \underbrace{(-k_f^2)u(x,y)e^{i(k_f z)}}_{\text{Laplace for z dir.}} - k_f^2 n^2(x,y)e^{ik_f z}u(x,y) = 0$$

$$-\Delta xyu(x,y) - \underbrace{k_f^2(-1+n^2(x,y))}_{k^2(x,y)\text{with } k=k_0+\delta_k}u(x,y) = 0$$

$$-\Delta xyu(x,y) - k_0^2 u(x,y) = \underbrace{(2k_0\delta_k(x,y) + \delta_k^2(x,y))}_{\lambda}u(x,y)$$

(If we solve this equation we get the lowest order eigenmode.)