Weierstraß-Institut für Angewandte Analysis und Stochastik

Matheon MF 1 Workshop
Optimisation Software

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Optimisation of diffraction gratings with DIPOG

Leibniz Gemeinschaft

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Outline

- Diffractive Optical Elements
- Finite Element Simulation
- Inverse Problems
- Optimization of Optical Gratings
- Examples
- Summary

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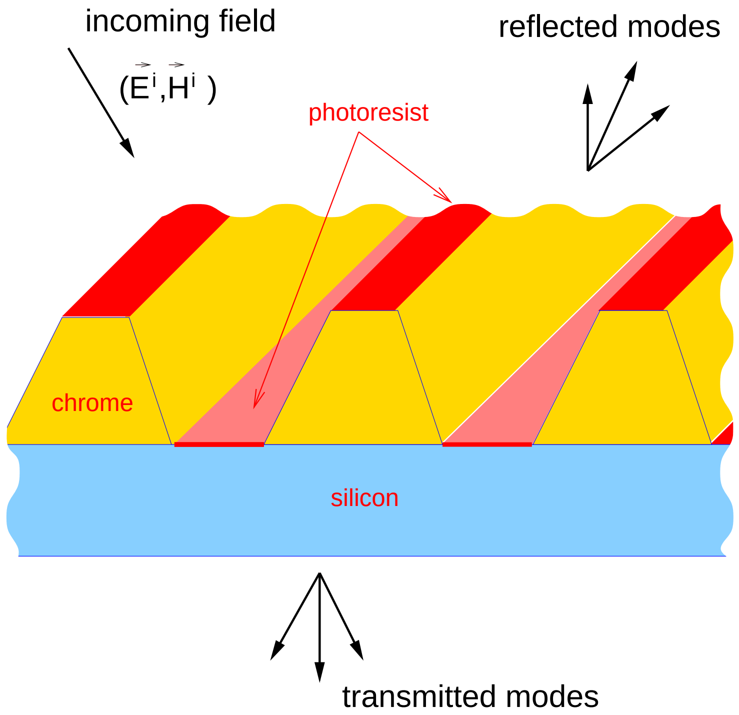
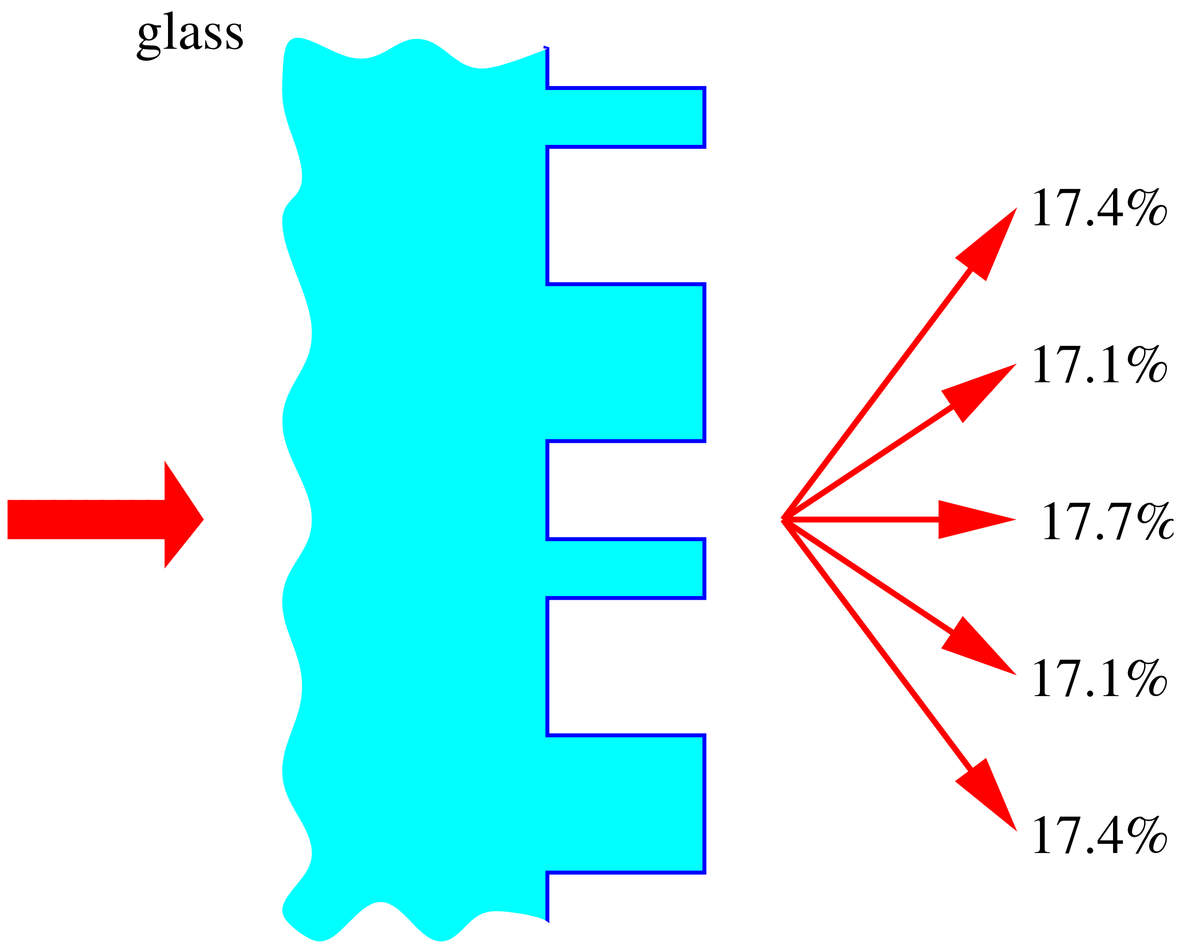
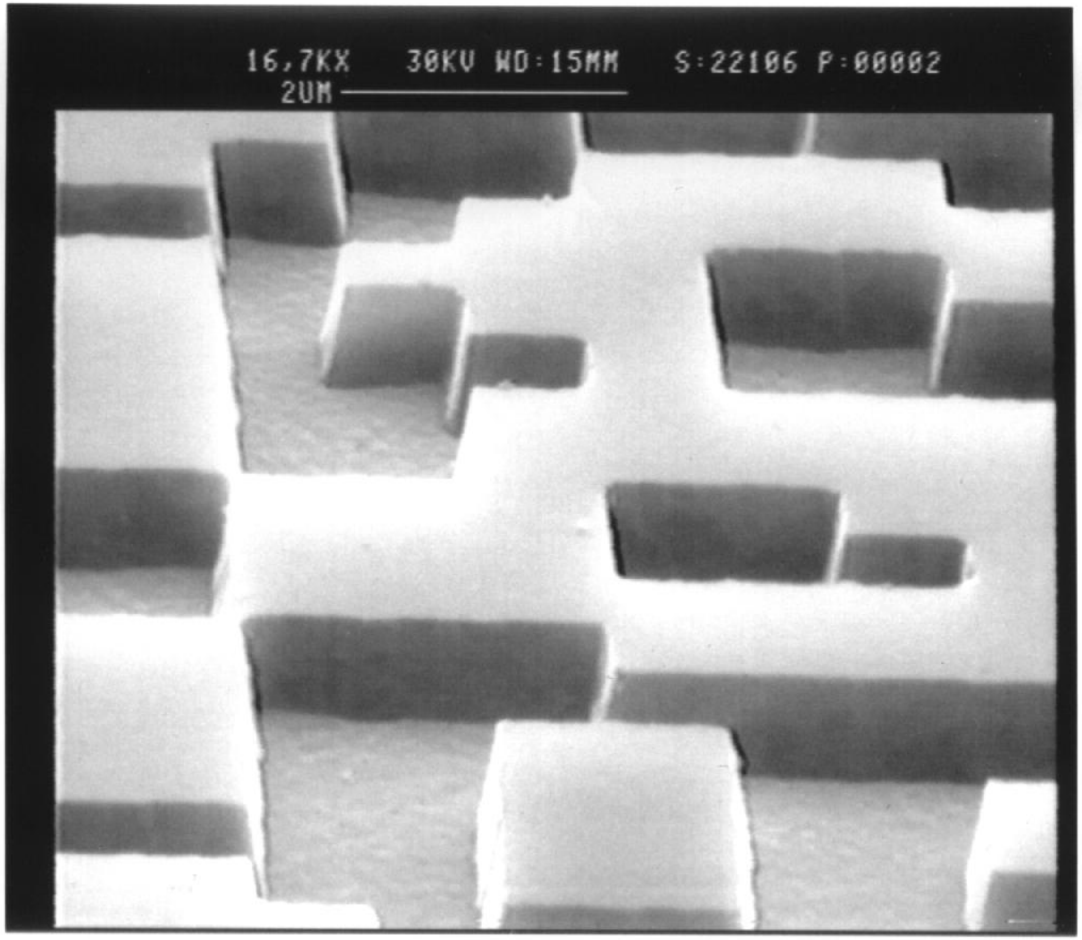


periodical grating (details of surface geometry in order of wavelength)



beam splitter



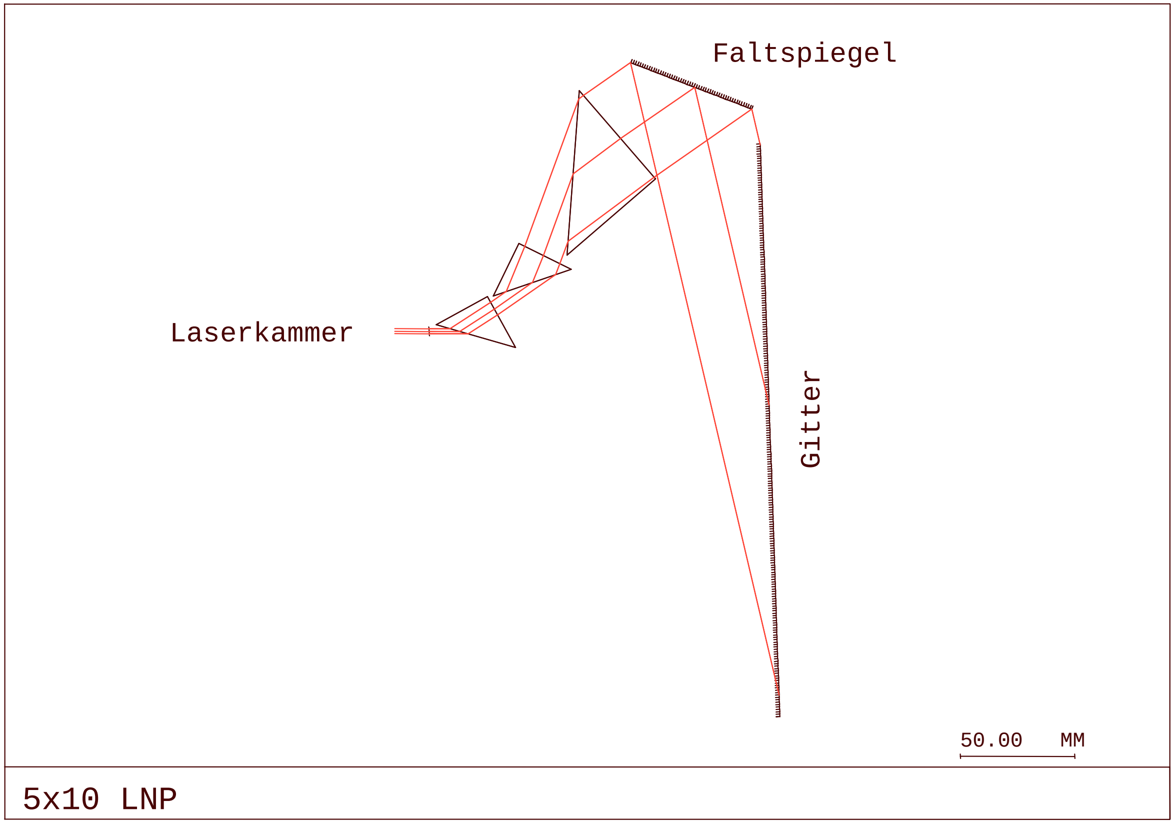
non-periodic grating, manufactured at BIFO

Microoptical and Other Diffractive Elements:

- ▷ realize old and new optical functions of optical devices
- ▷ e.g. by diffraction at surfaces and interfaces: forming and splitting of laser beams, diffraction and absorption
- ▷ smallest size resp. smallest details
- ▷ manufactured by means of semi-conductor industry, thin layer technology (photo resist exposition, try and wet etching, ion beam etching, vapor deposition)

more pictures from B. Kleemann (Carl Zeiss Oberkochen):

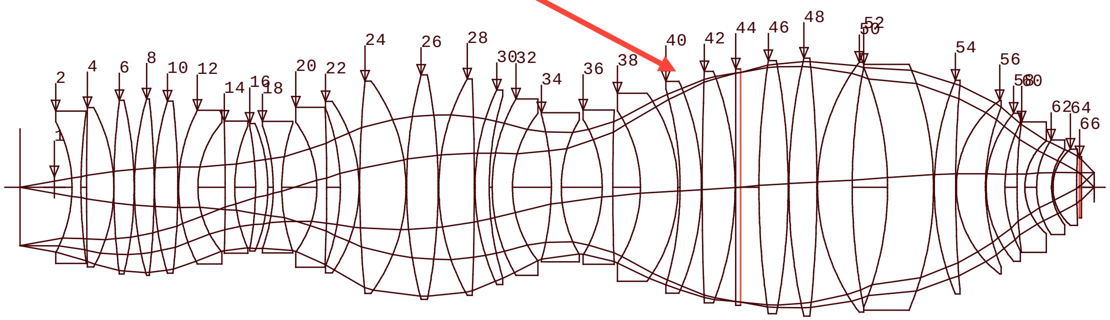
Einsatz des Laser-Gitters (Schema) in Littrow-Anwendung

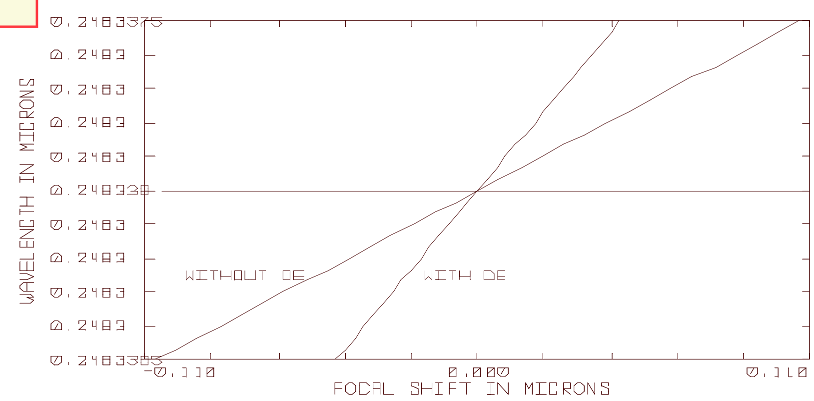


Diffraktive Linse in einem Projektionsobjektiv

Objektiv mit Diffraktiver Linse (DL)

λ = 248nm+/-0.5pm
NA = 0.7
Feld = 26x8mm^2
β' = -0.25
Material: Quarz
CHL = 0.2µm/pm
Bandbreite ~0.7pm





Objektiv mit DL:
CHL= 0.1µm/pm
Bandbreite~1.4pm
f_{DL}= 1250mm
d_{min}~ 3µm

Applications:

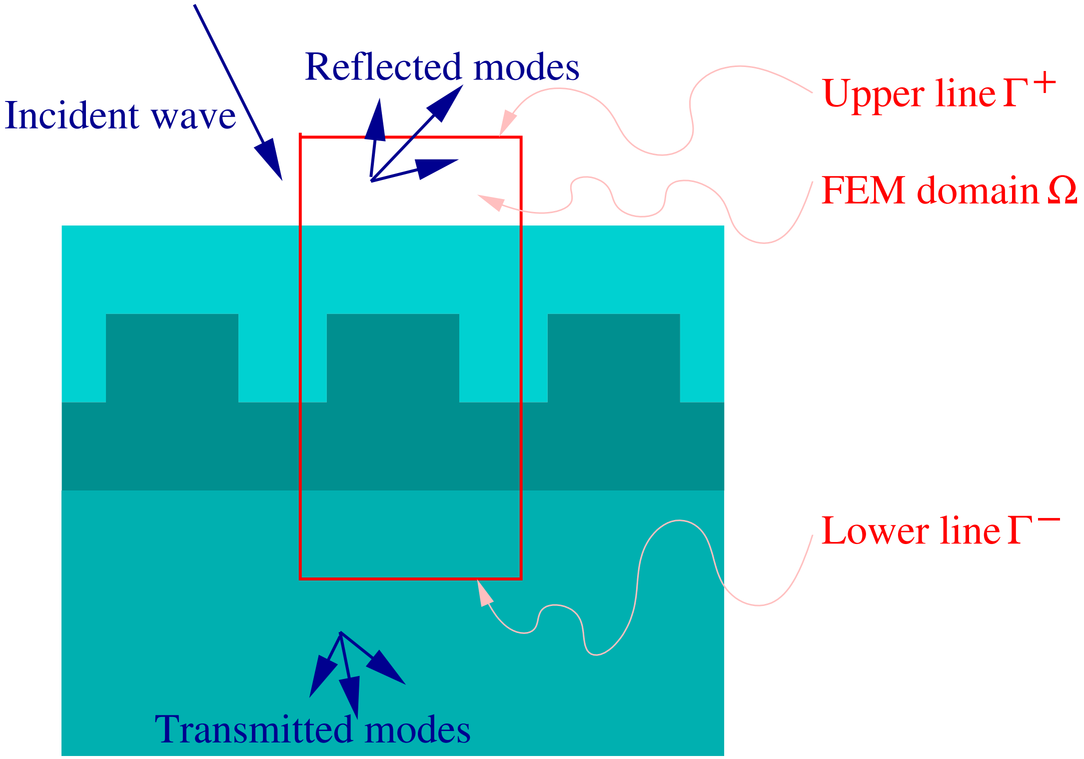
- ▷ Microscopy
- ▷ Spectroscopy
- ▷ Interferometry
- ▷ Correction of image abberations
- ▷ Wave forming elements (CGH)

Used in:

- ▷ Objectives for photography, microscopes, projectors
- ▷ Microelectronic circuits
- ▷ Solar technique
- ▷ Optical image processing
- ▷ Laser technique (data storage)
- ▷ Document security

Simplest example:

TM polarization (magnetic field orthogonal to cross section plane)
classical diffraction (incoming wave in cross section plane)



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Maxwell‘s equations $\longrightarrow$ problem reduces to scalar Helmholtz equation for transversal component v of amplitude of time harmonic magnetic field vector $v(x_1, x_2)\exp(-\mathbf{i}\omega t)$

$$\Delta v(x_1, x_2) + k^2 v(x_1, x_2) = 0, \quad k := \omega\sqrt{\mu\varepsilon}$$

where: ε electric permitivity
μ magnetic permeability
ω circular frequency of incoming light
k wavenumber

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Helmholtz equation fulfilled in domains with constant (contin.) wavenumber k
transmission condition through interfaces between different materials (continuous function, jump of derivative)

Floquet's theorem: Incoming plane wave of the form $\exp(\mathbf{i}\alpha x_1 - \mathbf{i}\beta x_2)$ leads to a quasi-periodic solution.

$$v(x_1 + d, x_2) \quad = \quad v(x_1, x_2) \exp(\mathbf{i}\alpha d)$$

where: d period of grating

$\alpha := k^+ \sin\theta$, θ angle of incidence

$\beta := k^+ \cos\theta$

k^+ wavenumber of cover material (air)

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k^+ wavenumber of cover material (air)

$$\begin{aligned} v(x_1, x_2)\exp(-\mathbf{i}\alpha x_1) &= \sum_{j=-\infty}^{\infty} c_j(x_2)\exp(\mathbf{i}j\frac{2\pi}{d}x_1), \\ v(x_1, x_2) &= \sum_{j=-\infty}^{\infty} A_j^+ \exp(\mathbf{i}\alpha_j x_1 + \mathbf{i}\beta_j^+ x_2) + \exp(\mathbf{i}\alpha x_1 - \mathbf{i}\beta x_2) \\ & \qquad x_2 > x_{max} \end{aligned}$$

.

$$v(x_1,x_2) = \sum_{j=-\infty}^{\infty} A_j^- \exp(\mathbf{i}\alpha_j x_1 - \mathbf{i}\beta_j^- x_2), \quad x_2 < x_{min}$$

$$\alpha_j := k^+ \sin(\theta) + \frac{2\pi}{d} j, \quad \beta_j^{\pm} := \sqrt{[k^{\pm}]^2 - [\alpha_j]^2}$$

Rayleigh series with Rayleigh coefficients $A_j^{\pm}$
Efficiency $e_j^{\pm}$ of j^{th} mode: rate of energy radiated into direction of mode

$$e_j^{\pm} := (\beta_j^{\pm}/\beta_0^{+})|A_j^{\pm}|^2$$

boundary condition for Helmholtz equation:
left and right boundary line: quasi-periodicity
upper and lower boundary line: derivative of solution in x_2 direction equals
. x_2 derivative of Rayleigh expansion

$$\int_\Omega \frac{1}{k^2}\{\nabla + \mathbf{i}(\alpha,0)\}u \cdot \overline{\{\nabla + \mathbf{i}(\alpha,0)\}\varphi} - \int_\Omega u\overline{\varphi} + \frac{1}{(k^+)^2}\int_{\Gamma^+}(T_\alpha^+ u)\overline{\varphi}$$
$$+\frac{1}{(k^-)^2}\int_{\Gamma^-}(T_\alpha^- u)\overline{\varphi} = -\frac{1}{(k^+)^2}\int_{\Gamma^+}(2\mathbf{i}\beta e^{-\mathbf{i}\beta x_2})\overline{\varphi}, \quad \varphi \in H^1_{per}(\Omega)$$

$$\mathbf{a}(u,\varphi) \;=\; \mathbf{F}(\varphi), \quad \varphi \in H^1_{per}(\Omega)$$

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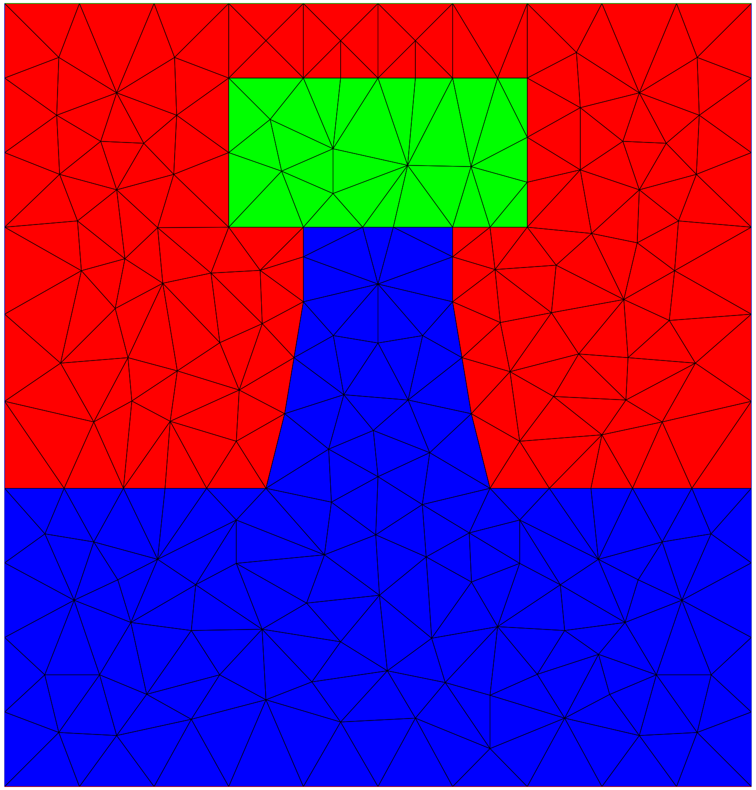
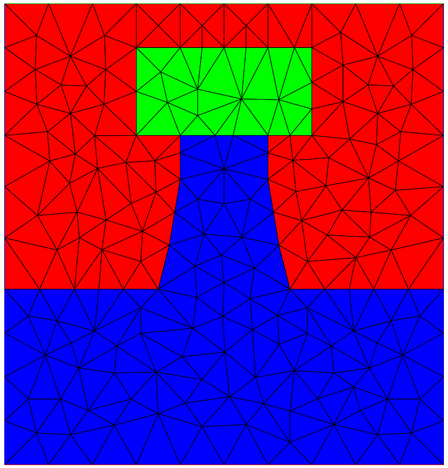
Triangulation (Shevchuk):





red: Air
green: resist
blue: SiO_2
Wavel.: 633 nm
Polariz.: TM
Angle inc.: 40°
Period: 1.7 μm

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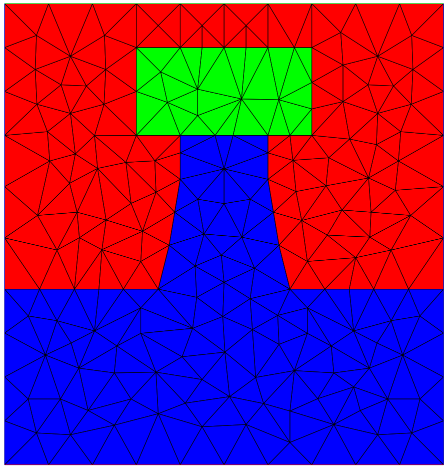

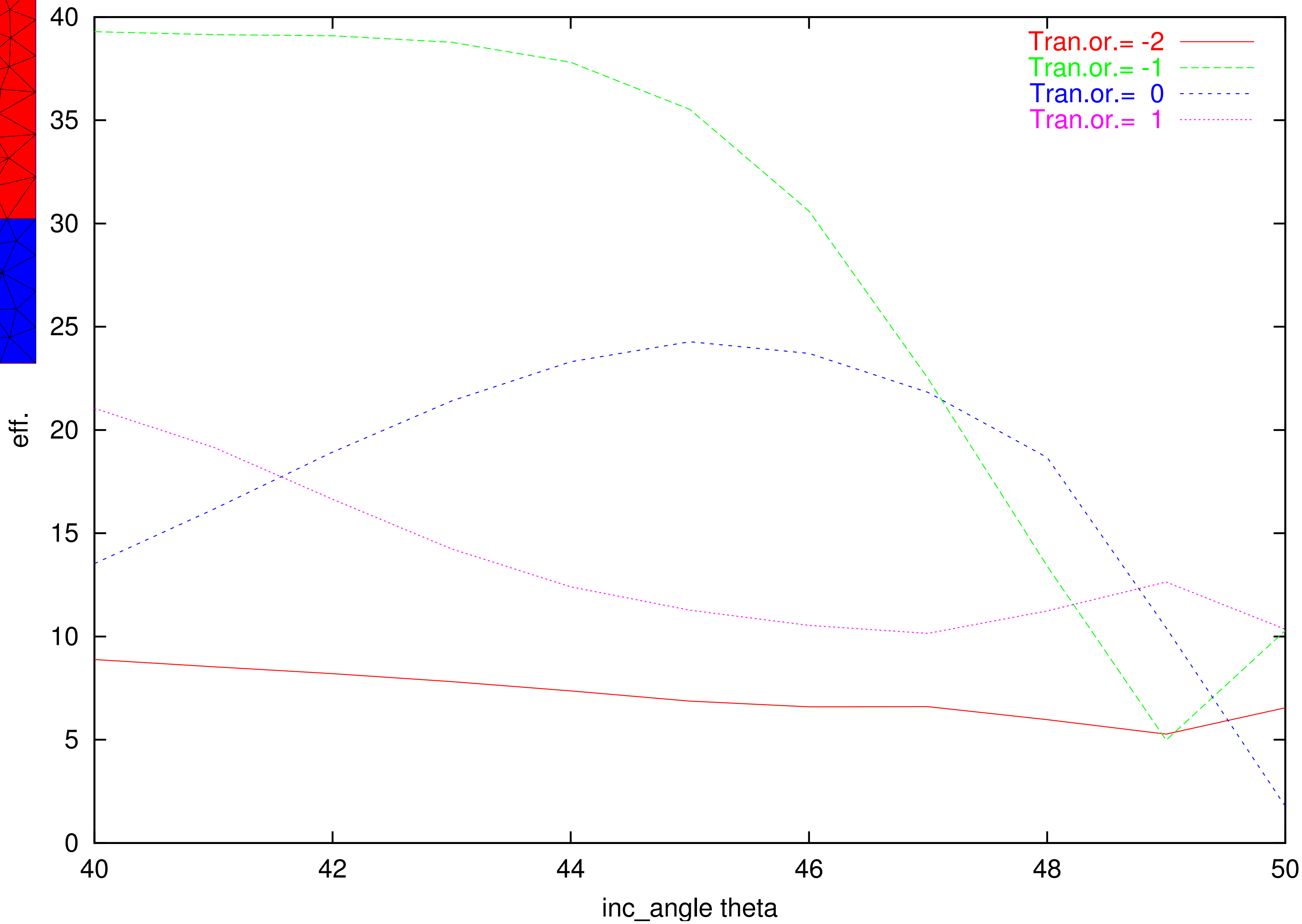

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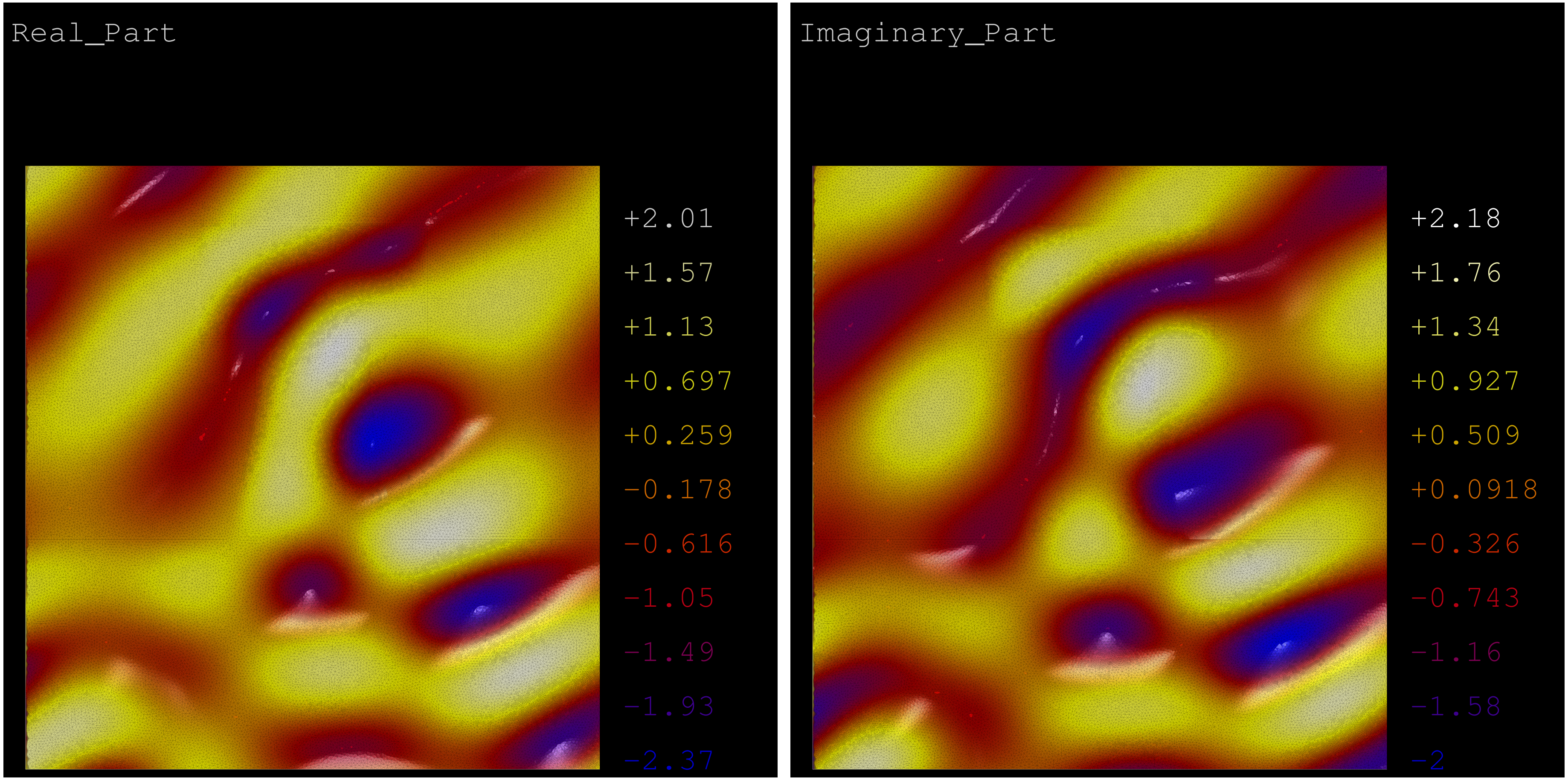
Finite Element Simulation



DIPOG:

- ▷ Program package for numerical solution of direct and inverse problems for optical gratings

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- FEM based on program package PDELIB of our institute

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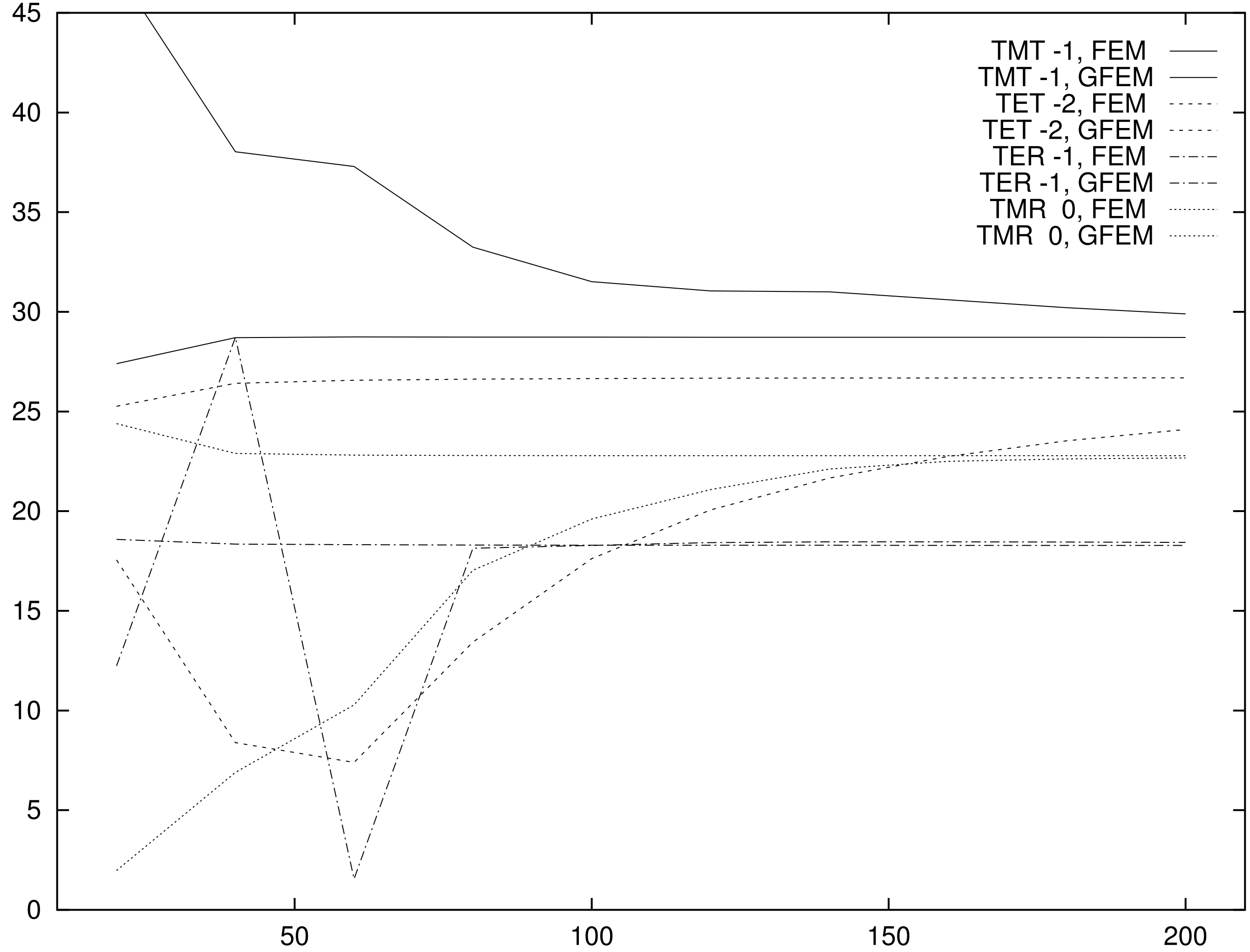
DIPOG:

- ▷ Program package for numerical solution of direct and inverse problems for optical gratings
- ▷ FEM based on program package PDELIB of our institute
- ▷ Rigorous treatment of outgoing wave condition by coupling with boundary elements
- ▷ Treatment of large wavelength (i.e.: many wavelengths λ over period d) by generalized FEM
  - – Generalized FEM due to Babuška/Ihlenburg/Paik/Sauter over uniform rectangular grids
  - – special combination of local Helmholtz solution as trial functions (cf. Partition of Unity Method by Babuška/Melenk or ultra-weak approach by Cessenat/Despres)
- ▷ Optimization



Efficiency (energy percentage) in dependence of DOF in one dim. simple binary grating discretized by uniform rectangular partition, comparison of conventional FEM with generalized GFEM

Application: quality check

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given:
measured farfield data = energy ratio and phase shifts (i.e. Rayleigh coefficients) of propagating reflected and transmitted modes under different angles of incidence resp. under different wavelengths

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Grating (represented e.g. by profile curve or by space dependent function of refractive index) which realizes the prescribed farfield data

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Inverse Problems (Reconstruction of gratings)

Application: quality check

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Grating (represented e.g. by profile curve or by space dependent function of refractive index) which realizes the prescribed farfield data

challenging mathematical problem: severely ill posed inverse problem
theoretical investigations: Uniqueness, Stability of Solution, Convergence of numerical algorithms

.

$$\mathcal{F}(k,u_1,\dots,u_L;\gamma) \;:=\; c_1\sum_{l=1}^{L}\left\|\widetilde{B}^{-1}\left[B(k,\theta_l)u_l - w_l\right]\right\|^2_{L^2(\Omega)} +$$
$$c_2\sum_{l=1}^{L}\|F(\theta_l)\,u_l - A_{meas}(\theta_l)\|^2_{\ell^2} \;+\gamma\left\{c_3\left\|k^2\right\|^2_{H^{1/2}_{per}(\Omega)} + c_4\sum_{l=1}^{L}\|u_l\|^2_{H^1_{per}(\Omega)}\right\}$$

arguments of obj.functional: Wavenumber function k and field functions $u_l,\ l=1,\dots,L$ for different angles of incidence

Regularization parameter: γ

precond.Helmholtz equ.: $\widetilde{B}^{-1}\left[B(k,\theta_l)u_l - w_l\right]$

Difference of farfield data: $F(\theta_l)u_l - A_{meas}(\theta_l)$ with measured data $A_{meas}(\theta_l)$ and data $F(\theta_l)u_l$ corresponding to u_l

.

$$
\begin{aligned}
\mathcal{F}(k, u_1, \dots, u_L; \gamma) \quad &\longrightarrow \quad \min \\
k^2 \in H^{1/2}_{per}(\Omega), & \\
u_l \in H^1_{per}(\Omega),\ l = 1, \dots, L &
\end{aligned}
$$

Discretization by FEM $\longrightarrow$ finite dimensional problem
Method of conjugate gradients for optimization
(resp. SQP method for a modified object.function)

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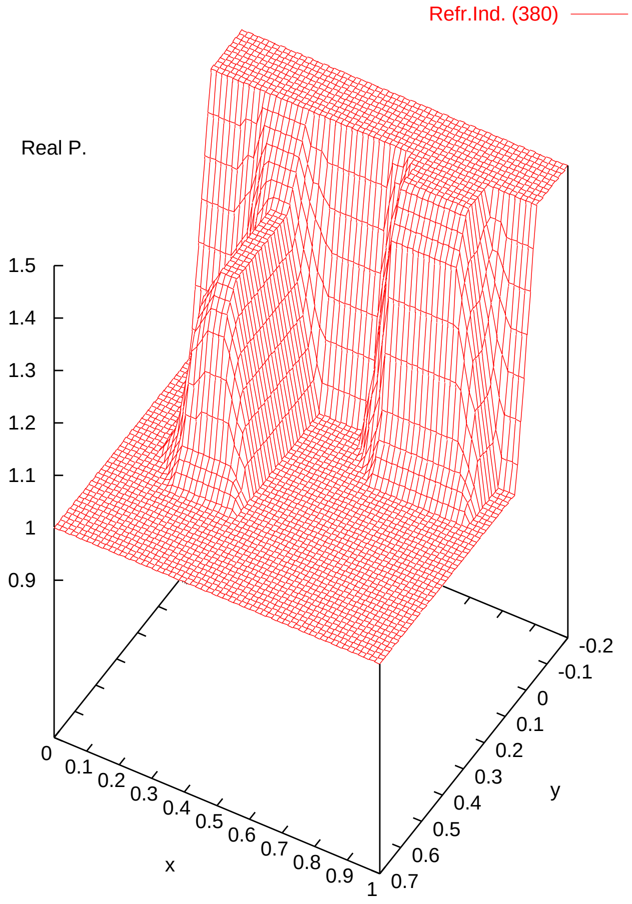
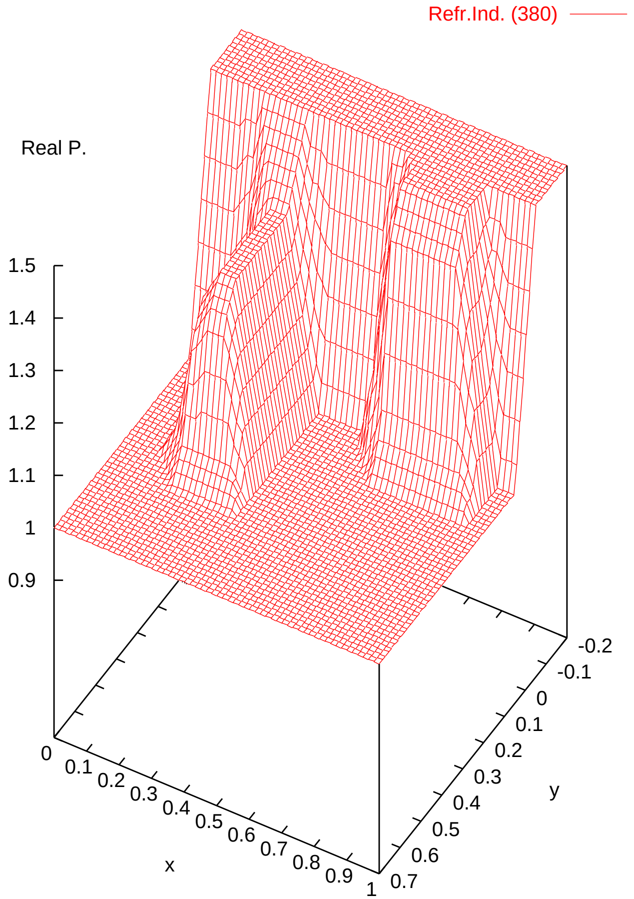
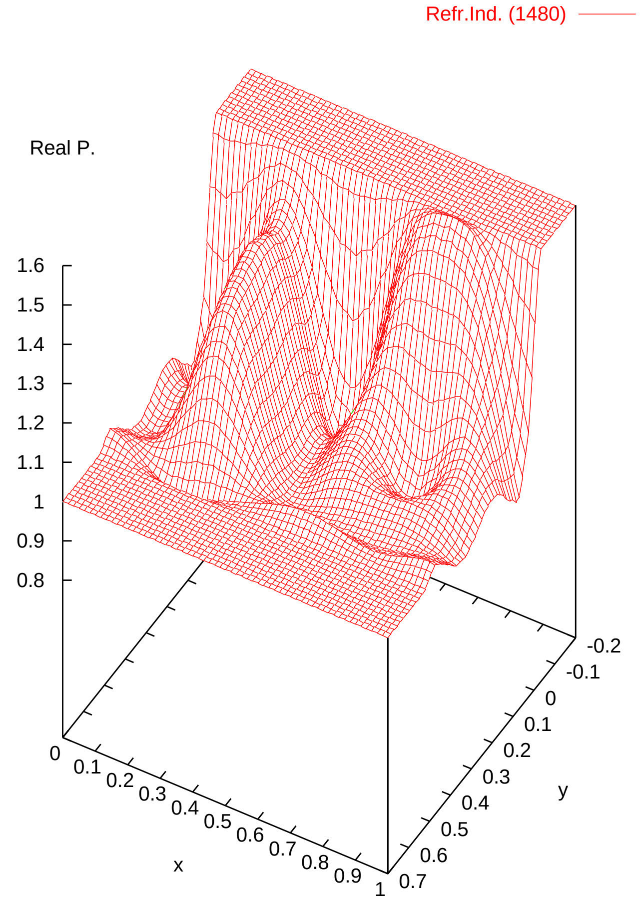
Example:

Number of angles of incidence:	$L = 25$
Degr.of Freedom of FEM:	L times $1\,600$
Degr.of Freedom for k:	400



prescribed function k over cross section of grating





prescribed function k over cross section of grating and reconstructed function k

- ▷ Inverse problems with a restricted number of geometry parameters (difficult ill posed problem turns into “simple” well posed problem)
- ▷ Design problem: design grating to realize a desired farfield pattern

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▷ Design problem: design grating to realize a desired farfield pattern

Objective functional:

$$\Phi\Big(e_j^{\pm}(\lambda_m,\theta_n), A_j^{\pm}(\lambda_m,\theta_n)\Big) \longrightarrow \inf$$

$$\Phi\Big(e_j^{\pm}(\lambda_m,\theta_n), A_j^{\pm}(\lambda_m,\theta_n)\Big) \overset{\text{e.g.}}{=} \sum_{\lambda_m,\theta_n} \Big| e_j^{\pm}(\lambda_m,\theta_n) - e_{j,\text{desired}}^{\pm}(\lambda_m,\theta_n)\Big|^2$$

.

Optimization parameters:

- ▷ Widths, heights, and position of rectangles in (multi-layered) binary grating
- ▷ Coordinates of polygonal profile (interface of two material regions)
- ▷ Refractive indices of material

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Mathematical properties of problem:

- ▷ objective functional: non-linear and smooth (FEM discretization even discont.)
- ▷ domain: lower dimensional box
- ▷ constraints: eventually many non-linear smooth functionals
- ▷ computation of function and gradient: time consuming

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Optimization methods:

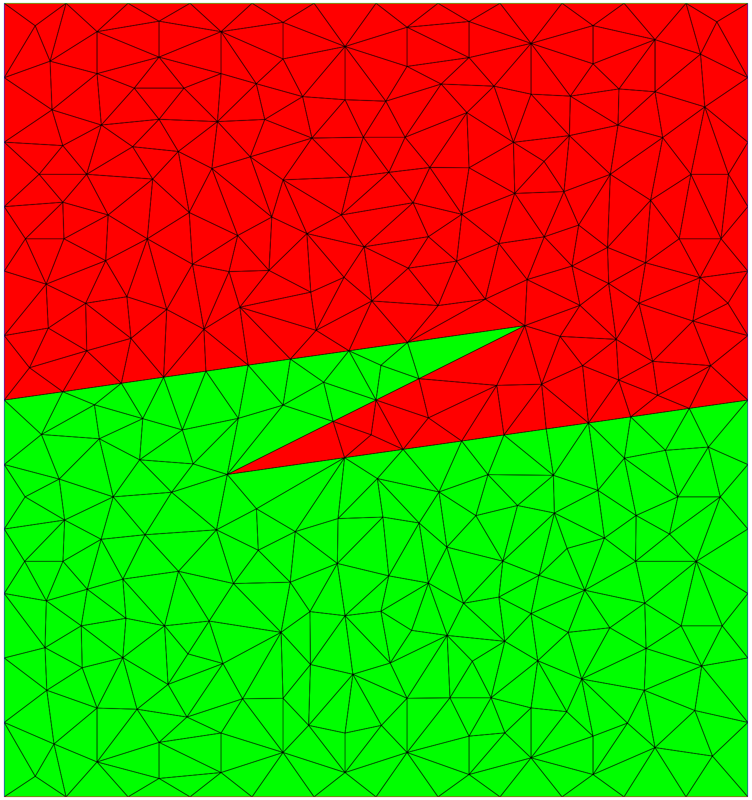
- ▷ global method (Simulated annealing)
- ▷ gradient based methods (Interior point method, Method of conjugate gradients, Augmented Lagrangian method)
- ▷ gradients: integral representation including solution of dual problem or representation by solution of original variational equ. with new right-hand side
- ▷ discretization of gradient via FEM

$$\mathbf{a}\left(\tilde{u},\varphi\right) \;=\; \mathbf{F}_{u,\chi}(\varphi), \qquad \varphi\in H^1_{per}(\Omega)$$

$$\begin{aligned}\mathbf{F}_{u,\chi}(\varphi) \;:=\; \frac{1}{k^2}\int_\Omega \Big\{ & k^2\nabla\chi\, u\overline{\varphi} + \partial_x\chi_y\left[(\partial_x u + \mathbf{i}\alpha u)\,\overline{\partial_y\varphi} + \partial_y u\overline{(\partial_x\varphi + \mathbf{i}\alpha\varphi)}\right] \\ & +\partial_y\chi_x\left[\partial_x u\overline{\partial_y\varphi} + \partial_y u\overline{\partial_x\varphi}\,\right] \\ & -\partial_x\chi_x\left[\partial_y u\overline{\partial_y\varphi} - \partial_x u\overline{\partial_x\varphi} + \alpha^2 u\overline{\varphi}\right] \\ & -\partial_y\chi_y\left[(\partial_x u + \mathbf{i}\alpha u)\,\overline{(\partial_x\varphi + \mathbf{i}\alpha\varphi)} - \partial_y u\overline{\partial_x\varphi}\right]\Big\}\end{aligned}$$

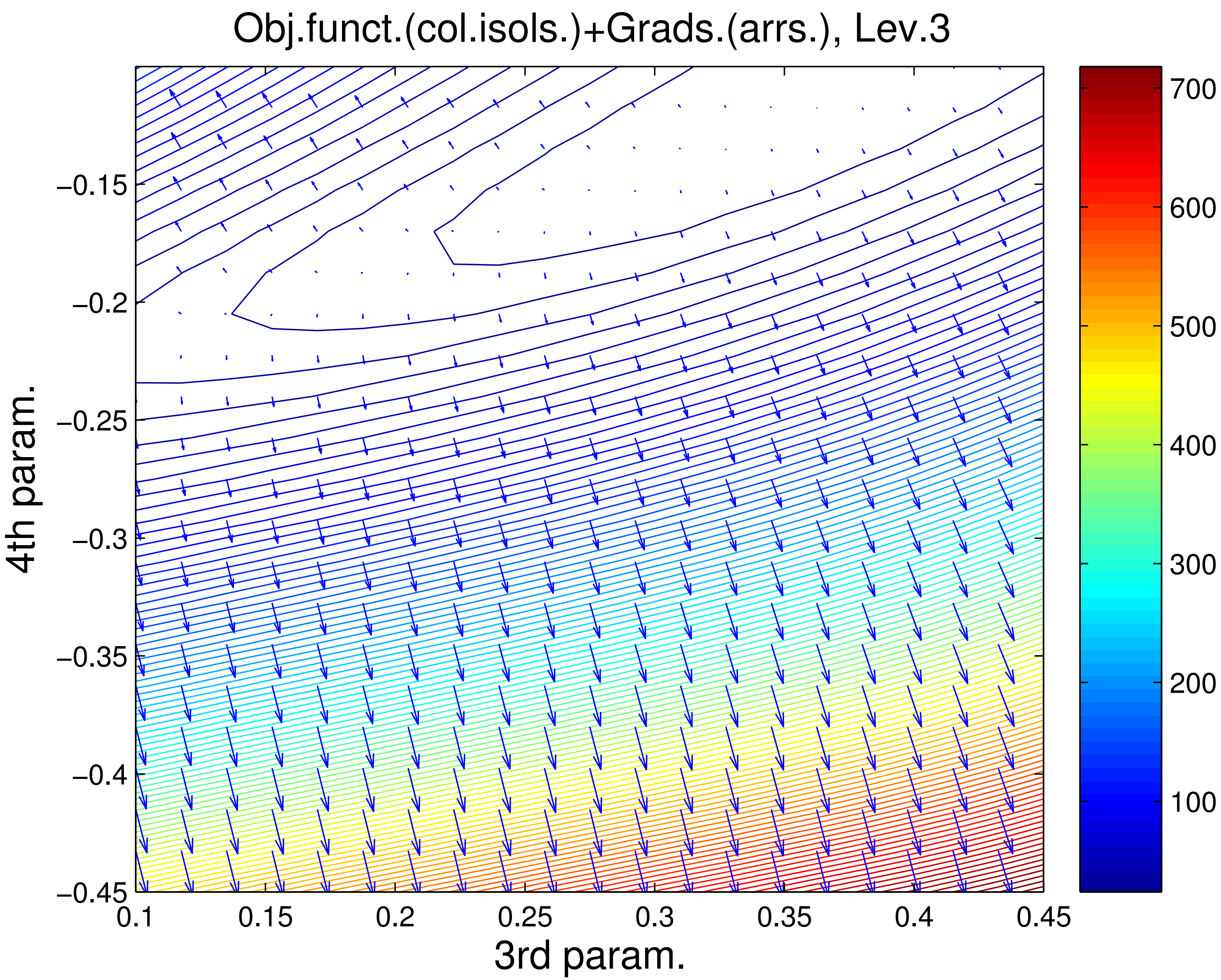
$$\frac{\partial A_j^{\pm}(u)}{\partial p} \;=\; A_j^{\pm}(\tilde{u})$$

where p is a coordinate of a corner point c at the polygonal interface and where χ is some cut off function of corner point c (piecewise linear at interface, one at c, zero over $\Gamma_\pm$)



simple polygonal grating: 3^{rd} and 4^{th} component of gradient (conical illumination)

$$\Phi = 0.004(e_0^{\mathrm{tr}} - 43.645)^2 + 0.004(e_{-1}^{\mathrm{tr}} - 43.247)^2 + 2.1(e_{-1}^{\mathrm{re}} - 2.141)^2 + 50(p_0^{\mathrm{tr}} - 48.10)^2 + 1200(p_{-1}^{\mathrm{tr}} - 44.36)^2 + 25(p_{-1}^{\mathrm{re}} - 17.29)^2$$


Obj.funct.(col.isols.)+Grads.(arrs.), Lev.3
4th param.
3rd param.
−0.15
−0.2
−0.25
−0.3
−0.35
−0.4
−0.45
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
700
600
500
400
300
200
100

Simple example

wavelength: λ=625 nm
period: 0 μm$\leq$x$\leq$1.5 μm
bounds for y-coordinates: -0.65 μm$\leq$y$\leq$0.65 μm
cover material: Air
refractive index of substrate: n=1.45
grating: polygonal profile grating with four corners
direction of illumination: $D = (\sin\theta\cos\phi, -\cos\theta, \sin\theta\sin\phi)$, $\theta = 48°$, $\phi = 10°$
TE polarization: incident electric field $\perp$ wavevector and normal of grating plane
refl.efficiencies and phase shifts: TE polarized, i.e. projections onto $D \times (0,1,0)$
number of finite elements (DOF) at level 3: $\approx$ 8 000

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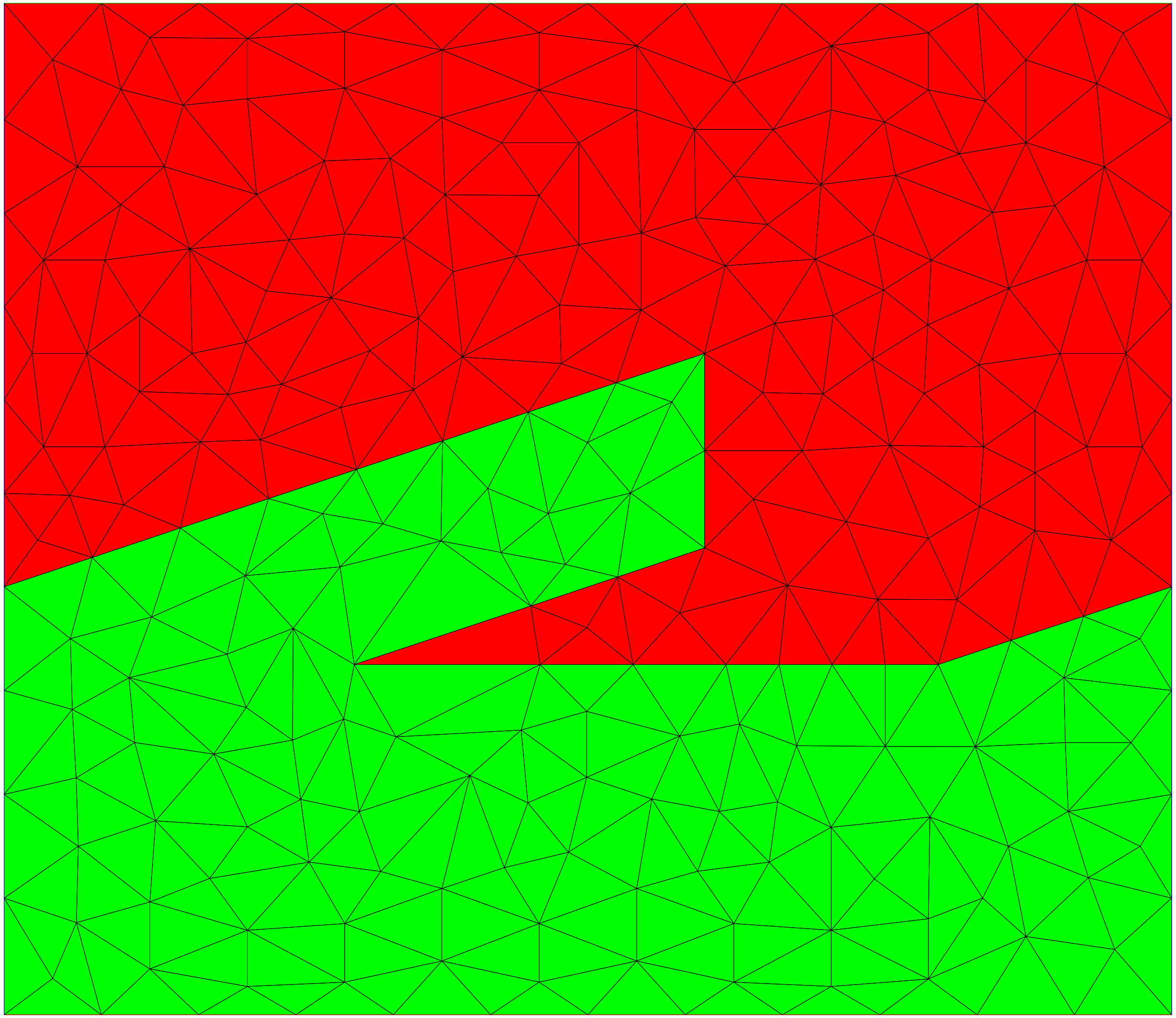
.

$$\Phi = \left|e_0^{re} - 45.87\right|^2 + 0.01\left|e_{-1}^{re} - 35.83\right|^2 + 1.5\left|p_0^{re} - 49.04\right|^2 + 3\left|p_{-1}^{re} - 74.08\right|^2$$

$\Phi = 0$ for high level simulation and for grating (which is to be reconstructed?):



Simulated annealing

cooling factor: 0.95

size of neighbourhood: 0.03

cooling steps: 150

restarts: 100

computing time: 3.75 h

value for solution: $\Phi = 0.5969$

.

Simulated annealing

cooling factor: 0.95
size of neighbourhood: 0.03
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restarts: 100
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value for solution: $\Phi = 0.5969$

Conjugate gradients

initial solution: (0.3,0.1), (0.6,0.2), (0.9,0.2), (1.2,0.1)
iterations: 138
number of computed gradients: 385
computing time: 5 min
value for solution: $\Phi = 0.2597 < 397.2$

.

Conjugate gradients

initial solution: solution of simulated annealing

iterations: 23

number of computed gradients: 89

value for solution: $\Phi = 0.5338 < 0.5969$

.

Examples

Conjugate gradients

initial solution: solution of simulated annealing

iterations: 23

number of computed gradients: 89

value for solution: $\Phi = 0.5338 < 0.5969$

Conjugate gradients

initial solution: exact sol.of higher level

iterations: 8

number of computed gradients: 51

value for solution: $\Phi = 0.002679 < 0.03467$

.

Examples

Conjugate gradients
initial solution: solution of simulated annealing
iterations: 23
number of computed gradients: 89
value for solution: $\Phi = 0.5338 < 0.5969$

Conjugate gradients
initial solution: exact sol.of higher level
iterations: 8
number of computed gradients: 51
value for solution: $\Phi = 0.002679 < 0.03467$

Conjugate gradients
initial solution: exact sol.+$\mathcal{O}(0.05)$
iterations: 23
number of computed gradients: 89
value for solution: $\Phi = 0.08845 < 120.77$
solution not recovered!

Conjugate gradients

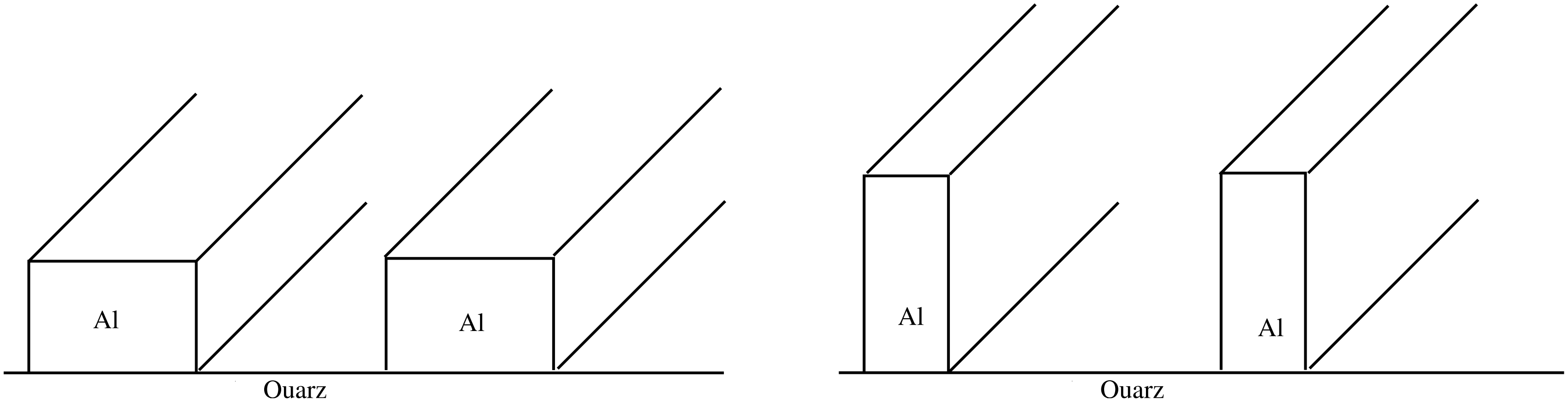
level: 2
initial solution: exact sol.+$\mathcal{O}(0.05)$
value for solution after 10 iterations: $\Phi = 0.20538 < 143.62$

level: 3
initial solution: solution of level 2
value for solution after 10 iterations: $\Phi = 0.31607 < 4.5271$

level: 4
initial solution: solution of level 3
value for solution after 10 iterations: $\Phi = 0.31607 < 4.4242$

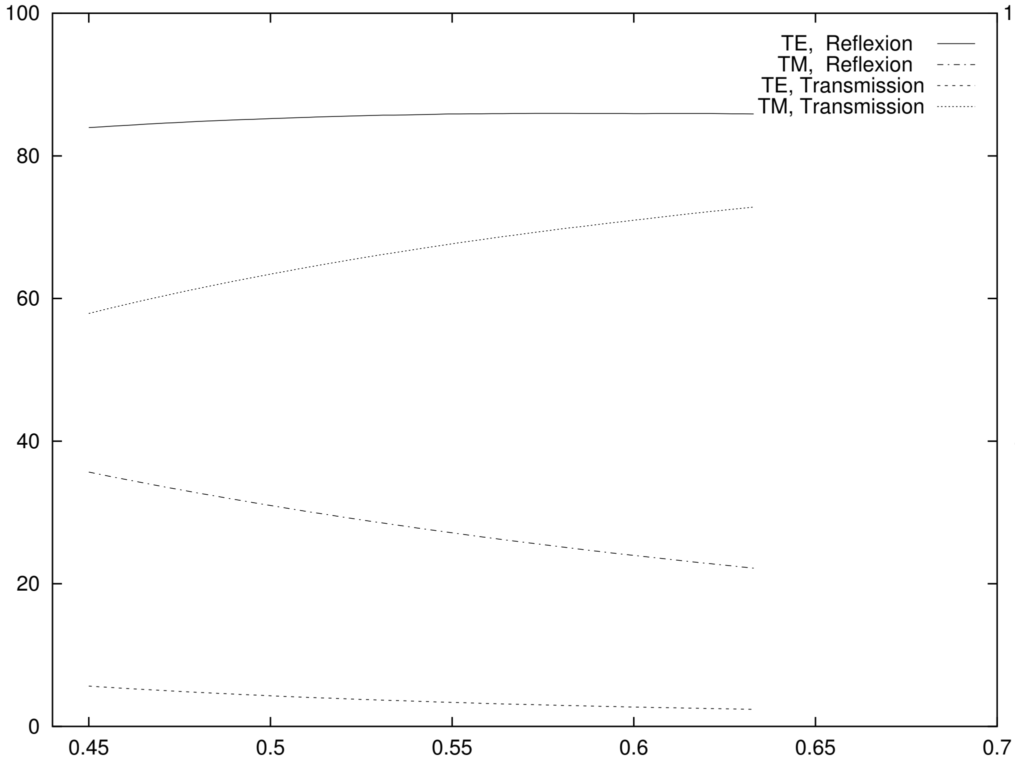
level: 5
initial solution: solution of level 4
value for solution after 10 iterations: $\Phi = 0.29093 < 0.3301$
value for solution after 100 iterations: $\Phi = 0.14013 < 0.3301$

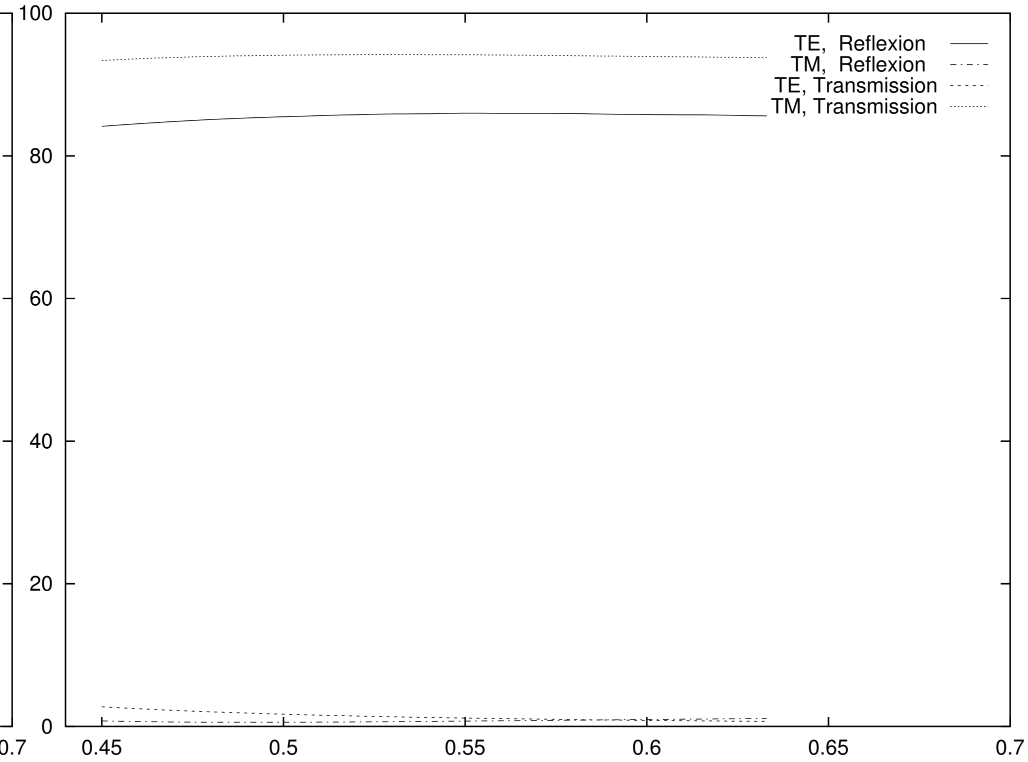
Examples



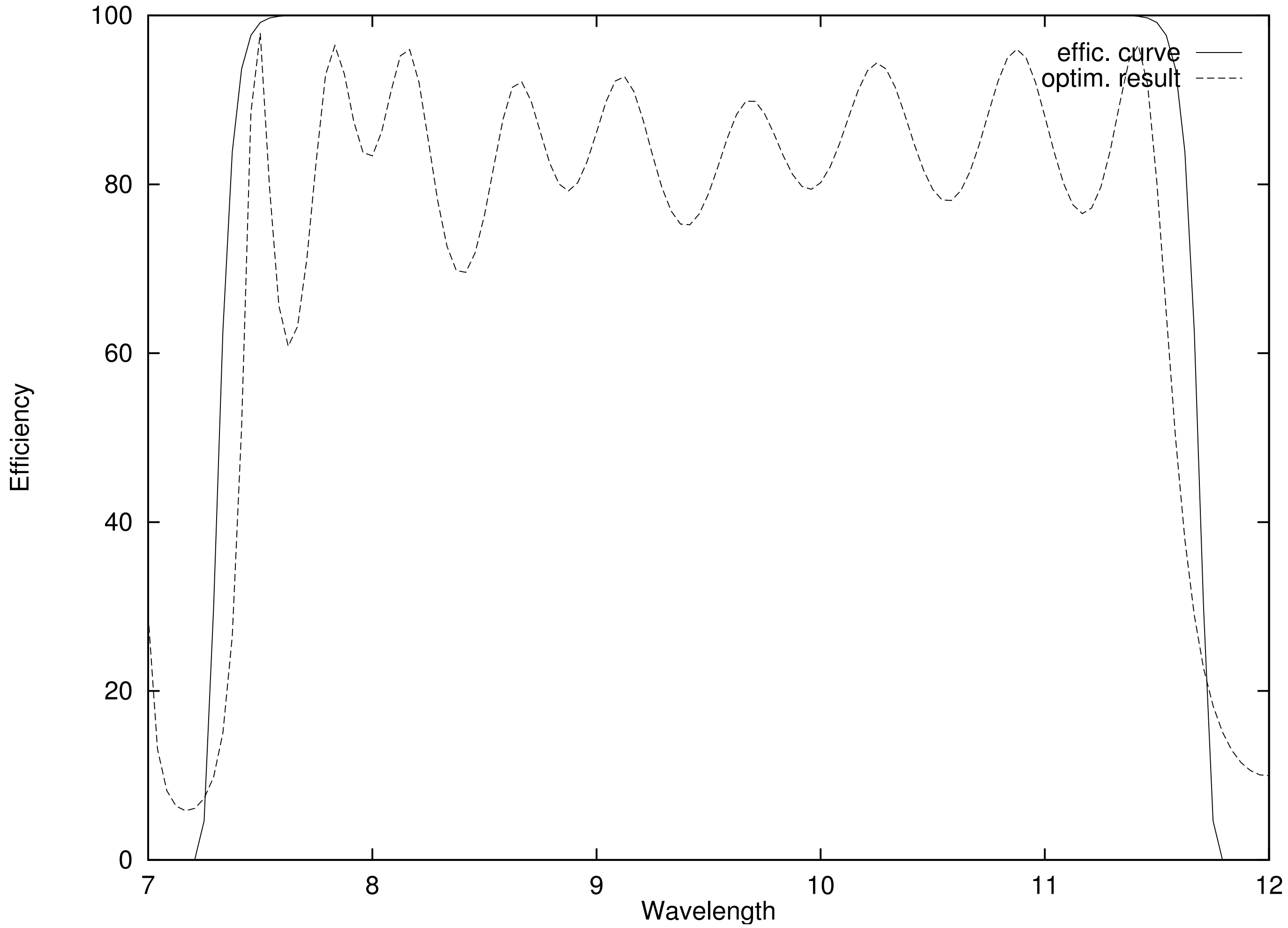
Initial and optimal solution for polarization grating

Examples

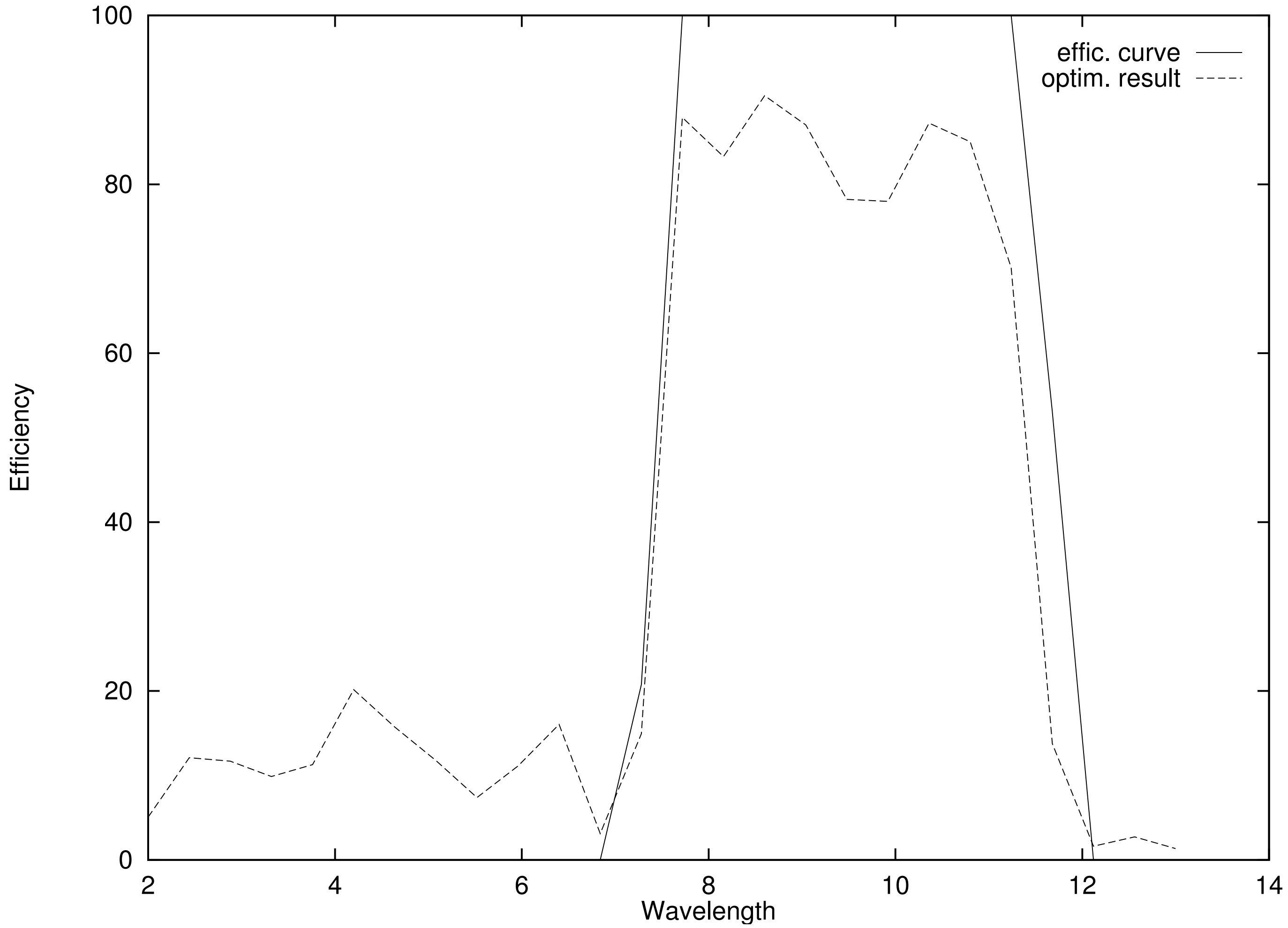




Polarization grating: TE light reflected, TM light transmitted



Optimization of 20 layers for maximization of transmitted energy



Optimization of additional binary grating over the 20 layers

Summary

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Summary

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  - – This is a rigorous method.
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- ▷ Algorithms useful for reconstruction problems and design of gratings. The corresponding DIPOG routines are still under development.
- ▷ Thank you for your attention.

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