Weierstraß-Institut für Angewandte Analysis und Stochastik

A. Rathsfeld

245th Seminar on Scatterometry and Ellipsometry on Structured Surfaces

Modelling and Algorithms for Simulation and Reconstruction in Scatterometry

joint work with: Hermann Groß

Physikalisch-Technische Bundesanstalt, Working Group 8.41,

"Modelling and Simulation"

Outline

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Fast schemes (geometrical optics, Kirchhoff approximation, etc.) not sufficiently accurate for polarization sensitive scattering by tiny objects! Solve time-harmonic Maxwell's equations with boundary conditions:

- Curl-Curl equation for three-dimensional amplitude factor of time harmonic electric field (i.e. $\mathcal{E}(x_1, x_2, x_3, t) = E(x_1, x_2, x_3)e^{-i\omega t}$)

$$\nabla \times \nabla \times E(x_1, x_2, x_3) - k^2 E(x_1, x_2, x_3) = 0, \;\; k := \omega\sqrt{\mu_0 \varepsilon_0}\, n$$

- scalar 2D Helmholtz equation if geometry is constant in x_3 direction and if direction of incoming plane wave is in x_1-x_2 plane

$$\Delta v(x_1, x_2) + k^2 v(x_1, x_2) = 0, \;\; v = E_3, H_3$$

- two coupled scalar 2D Helmholtz equations if geometry is constant in x_3 direction, direction not in x_1-x_2 plane

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Boundary value problems:

- conditions at boundary point with normal ν to boundary face

$$\nu \times E = \nu \times E^{\text{incident}}, \quad \nu \times \nabla \times E = \nu \times \nabla \times E^{\text{incident}}$$

- impedance boundary conditions, perfect conductor at boundary
- quasi-periodic boundary conditions including period p

$$E(x, y, z + p) = qE(x, y, z), \quad q := \frac{e^{\mathbf{i}\vec{k}\cdot(x,y,z+p)}}{e^{\mathbf{i}\vec{k}\cdot(x,y,z)}}$$

- coupling to solutions on outer domain satisfying the radiation condition: no incoming wave mode contained in coupled outer solution (represented as Rayleigh series or boundary integral)

Rigorous?

- Is Maxwell's system sufficient? Quantum physics needed?
- There will be errors in the numerical computation!

Variational equation

$$\int_\Omega \nabla \times E \cdot \overline{\nabla \times F} - \int_\Omega k^2 E \cdot \overline{F} + \int_\Gamma (TE) \cdot \overline{F} = -\int_{\Gamma+} E^{\text{incident}} \overline{F},$$

for all F in $H(\text{curl}, \Omega)$

$$\mathbf{a}(E, F) \;=\; \mathbf{b}(F), \quad \text{for all } F \text{ in } H(\text{curl}, \Omega)$$

with: T operator of boundary condition
Ω domain of computation (over one period)
$\Gamma \subseteq \partial\Omega$ non-periodic boundary faces
$H(\text{curl}, \Omega)$ solutions with finite energy

Finite element method (FEM)

Replace continuous functions E, F in variational equation by approximate functions from finite element space $\mathcal{F}_h(\Omega)$ which contains functions piecewise polynomial over a fixed FEM partition $\Omega = \cup_{j=1}^{J} \Omega_j$ with $\operatorname{diam} \Omega_j \leq h$

$$\int_\Omega \nabla \times E_h \cdot \overline{\nabla \times F_h} - \int_\Omega k^2 E_h \cdot \overline{F_h} + \int_\Gamma (TE_h) \cdot \overline{F_h} = - \int_{\Gamma^+} E_h^{\text{incident}} \overline{F_h},$$

for all F_h in $\mathcal{F}_h(\Omega)$

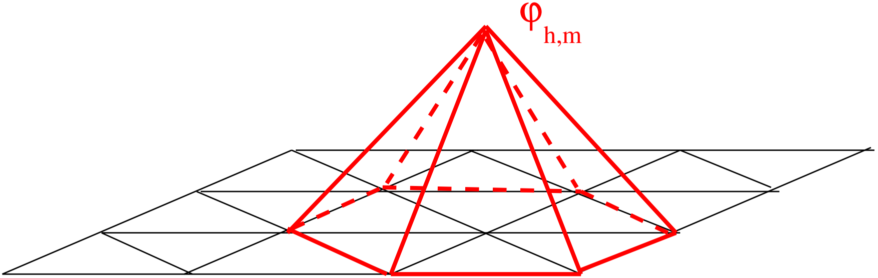
$$\mathbf{a}(E_h, F_h) \ = \ \mathbf{b}(F_h), \quad \text{for all } F_h \text{ in } \mathcal{F}_h(\Omega)$$

choose a natural finite element basis $(\varphi_{h,m})$ in $\mathcal{F}_h(\Omega)$,
FEM system is equivalent to matrix equation

$$E_h = \sum_{m=1}^{M} \xi_m \varphi_{h,m}$$

$$M(\xi_m) = (\eta_m), \; M = \left(\mathbf{a}\left(\varphi_{h,m}, \varphi_{h,m'}\right)\right)_{m,m'}$$

For Helmholtz equation, piecewise linear nodal basis over hexagonal two-dimensional mesh: hat function



For Curl-Curl equation, edge elements (Nédélec):

- noncontinuous piecewise linear (polynomial) functions
- better approximation of $\{E: \nabla \times \nabla \times E = 0\}$

$$\varphi_{h,e} \quad = \quad \varphi_{h,m} \nabla \varphi_{h,m'} - \varphi_{h,m'} \nabla \varphi_{h,m}, \qquad e = (m, m')$$

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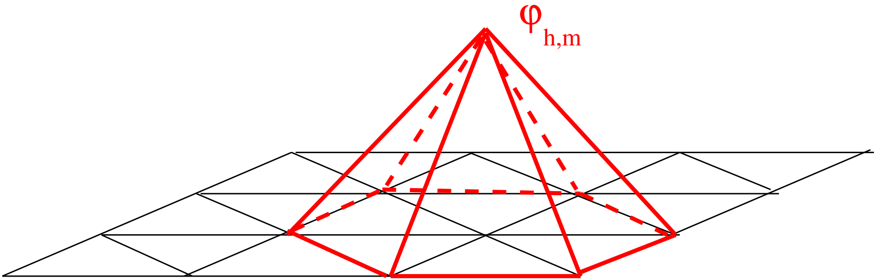

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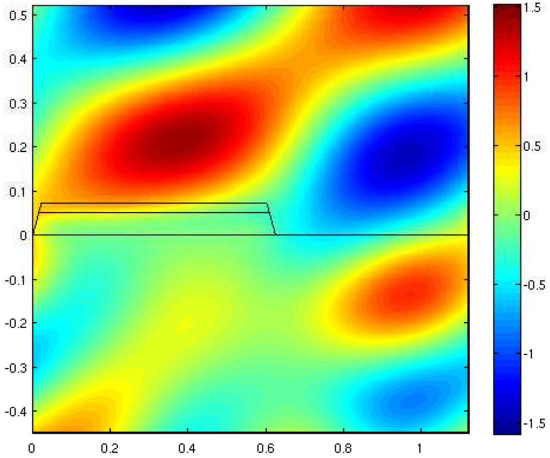
Radiation condition:

- Coupling with potential solution in outer region (boundary element method)
- Absorbing boundary conditions (PML, Bérenger): introduce artificial "absorbing" material surrounding the computational domain
- Mortaring with Fourier mode solutions: solution in outer region represented by superposition of Fourier mode solutions, weak boundary conditions enforced by penalty terms over boundary (Nitsche, Stenberg, Huber, Schöberl, Sinwel, Zaglmayr)

$$\mathbf{a}\left((E, E^{\mathrm{FM}}), (F, F^{\mathrm{FM}})\right) = \ldots + \int_\Gamma \nu \times (E - E^{\mathrm{FM}}) \cdot \overline{\nabla \times F^{\mathrm{FM}}} \mathrm{d}\Gamma + \ldots$$

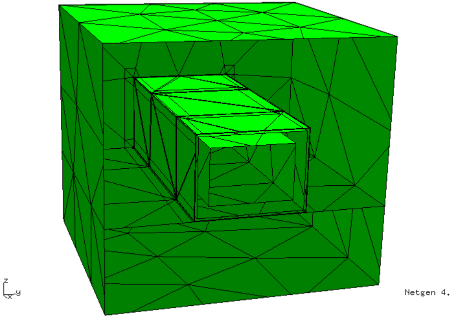
- Radiation condition for outer domain different from full or half space (Hohage, Schmidt, Zschiedrich)

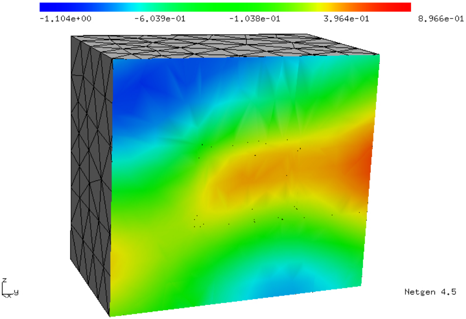

0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
0
0.2
0.4
0.6
0.8
1
1.5
1
0.5
0
-0.5
-1
-1.5

Component of electric field in groove direction

3D example

FEM grid and real part of x_1 component of electric field





Alternative methods:

- Finite Difference Methods (e.g. FDTD): similar to FEM, fast on regular grids
- Rigorous Coupled Wave Analysis (RCWA): solution approximated by truncated Fourier series expansion, domain split into slices, differential equation for vector of Fourier coefficients in the slice, S-Matrix propagation over the stack of slices
- Coordinate Transformation Method
- Differential Equation Methods
- Multipole Methods
- Integral Equation Methods (Boundary Element Methods): perfect for small number of boundaries and interfaces

General principle for all methods:

split domain in subdomains, solve in subdomains, couple particular solutions

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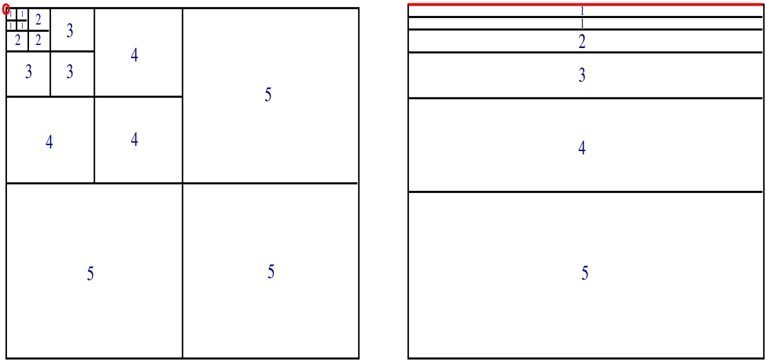
approximation of singularities and boundary layers

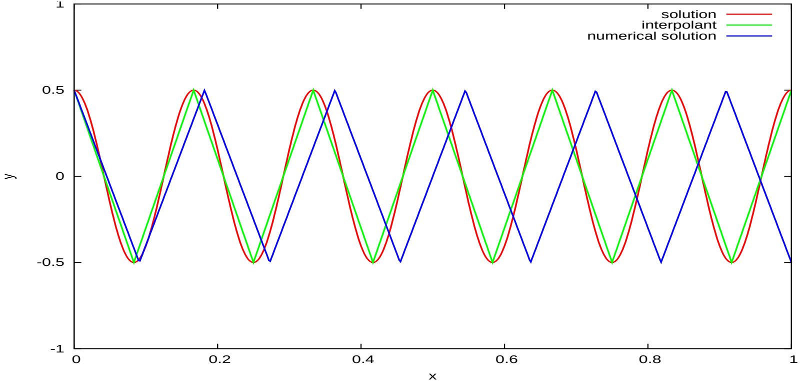


meshes graded toward singular points or towards interfaces

$h - p$ methods: variable polynomial degree of FE function

adaptive mesh generator controlled by local error estimator

Approximation of highly oscillating functions:



numerical dispersion (pollution):

- generalized finite elements
- high order finite elements
- non-sparse discretization scheme

Solver for huge systems of linear equations:

- ▷ Direct solver: slow, large amount of memory, stable solver
- ▷ Direct solver for sparse matrices: less memory, faster computation times, stable solver, good for 2D (Pardiso)
- ▷ Iterative solver
  - standard iteration without preconditioner: no convergence
  - multigrid method
  - domain decomposition (Schwarz method)
  - ultraweak formulation

No perfect solver has been found yet?

Outline

Full Inverse Problem:

- ▷ Given: the diffraction properties of structure (e.g. efficiencies $E^{\pm}_{j,l}$)
- ▷ Seek: the structure, i.e., the geometry of the domains filled with different materials and the refractive indices of these materials

- ◇ Diffraction limit: mathematically, a severely ill-posed problem, i.e. small errors in data lead to large errors for the solution
- ◇ contributions to mathematical 2D theory of gratings by F. Hettlich, A. Kirsch, G. Bruckner, J. Elschner, G. Schmidt, D.C. Dobson, G. Bao, A. Friedman, M. Yamamoto, J. Cheng, K. Ito, F. Reitich, and T. Arens
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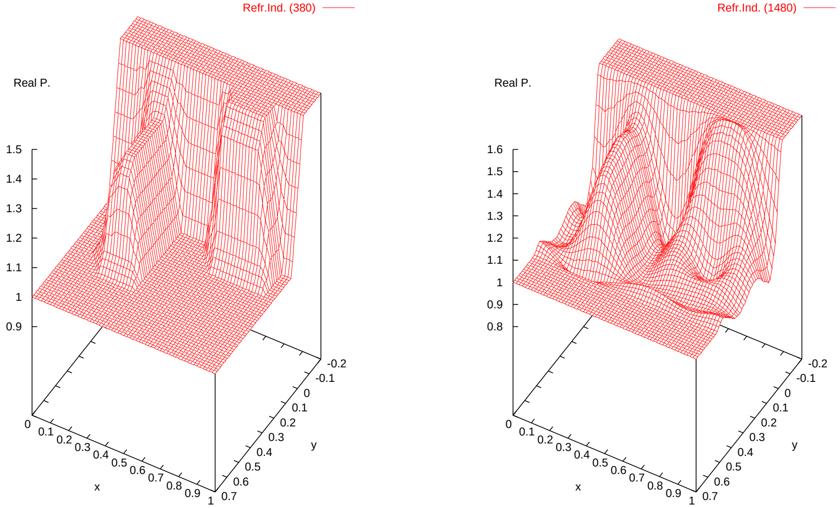
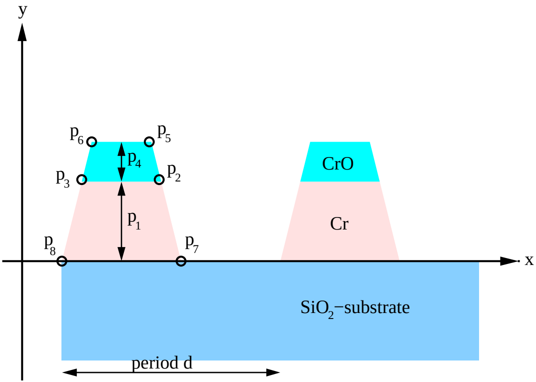


given and reconstructed refractive index over cross section of grating



$$h_i := p_i,\ i = 1,4, \quad h_i := \frac{p_i}{period},\ i = 2,5,7, \quad h_i := \frac{p_i}{p_{i-1}},\ i = 3,6,8$$

Operator Equation:

measured data, efficiencies or phase shifts: $E^{meas} = (E^{meas}_m)_{m\in\mathcal{M}}$
comp.data corresponding to parameters h: $E(h) = (E_m(h))_{m\in\mathcal{M}}$
constraints: $h_j^{min} \le h_j \le h_j^{max}$

$$E(h) \quad = \quad E^{meas}$$

Optimization Problem:

minimize objective functional

$$\Phi\Big(E_m(h)\Big) \longrightarrow \inf$$

$$\Phi\Big(E_m(h)\Big) \quad := \quad \sum_{m\in\mathcal{M}} \omega_m \left|E_m(h) - E_m^{meas}\right|^2$$

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Nonlinear, nonquadratic, nonconvex objective functional
time consuming evaluation of objective functional
simple box constraints
difficulty: find global minimum among several local minima

Global methods-stochastic methods:

- e.g. Simulated annealing
- e.g. Evolutionary (genetic) algorithms
- stochastic transitions of iterative solution (cooling step of particle system, adaption process of population of species)
- sufficiently large number of iterations: convergence to global minimum with probability one
- realistic number of iterations: heuristic method only

Faster methods:

precompute finite dimensional operator, e.g. generate a library of solution and search for solution in this library

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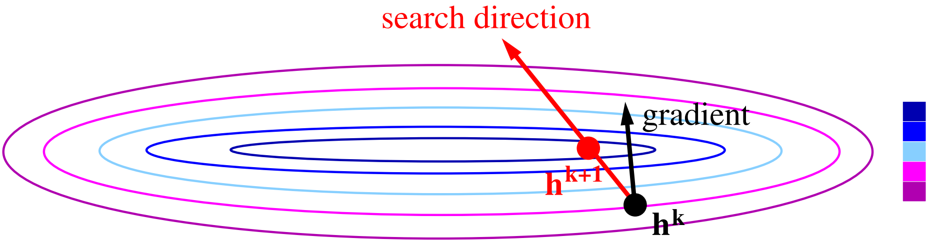
gradient based methods:

first order method with superlinear convergence:

- conjugate gradients method
- interior point method
- Levenberg-Marquardt algorithm
- Gauß-Newton method
- modification for box constraints: SQP type method

compute $h^{k+1} = h^k + \Delta h$ with Δh the optimal solution of convex quadratic optimization problem with box constraints:

$$\min_{\Delta h:\, h_j^{min} \leq [h_j^k + \Delta h]_j \leq h_j^{max}} \left\| E(h^k) + \frac{\partial E}{\partial h}(h^k)\Delta h - E^{meas} \right\|^2$$



gradient computation: search direction for new iterate h^{k+1}
line search for new iterate
new computations for objective functional required

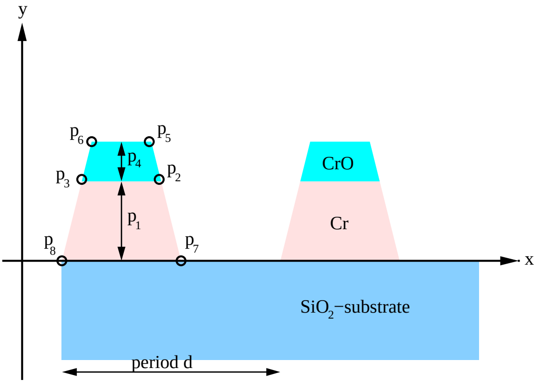
Gauß-Newton method or methods with second order derivatives yield
step size in search direction
however: line search algorithm is more stable

Scaling of Parameters and Measurement Values:

- Normalization factors for parameters: expected errors of parameters should correspond to uniform errors for normalized parameters
- Normalization factors for measurement values: measurement uncertainty should be the same for all normalized measurement values

$$\Phi\Big(E_m(h)\Big) := \sum_{m\in\mathcal{M}} \omega_m \left|E_m(h) - E_m^{meas}\right|^2$$

$$\omega_m \sim \frac{1}{u(E_m^{meas})^2}$$



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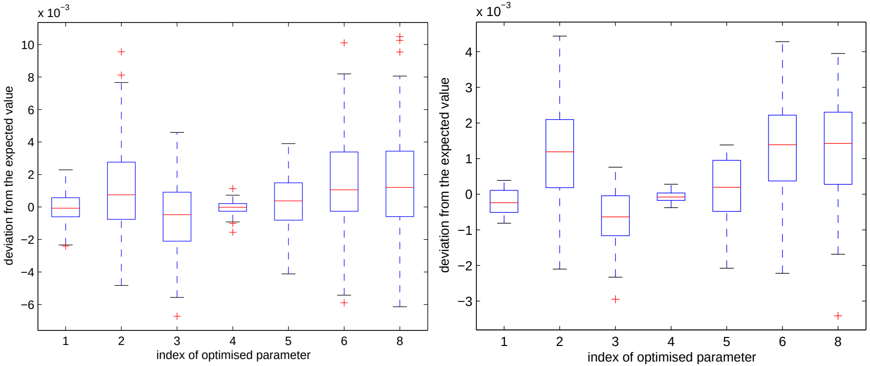
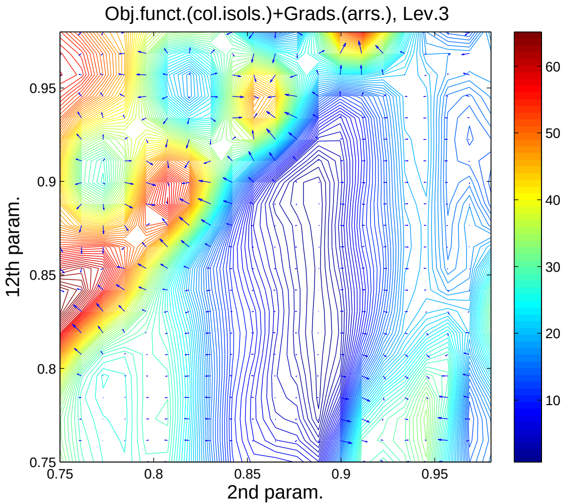
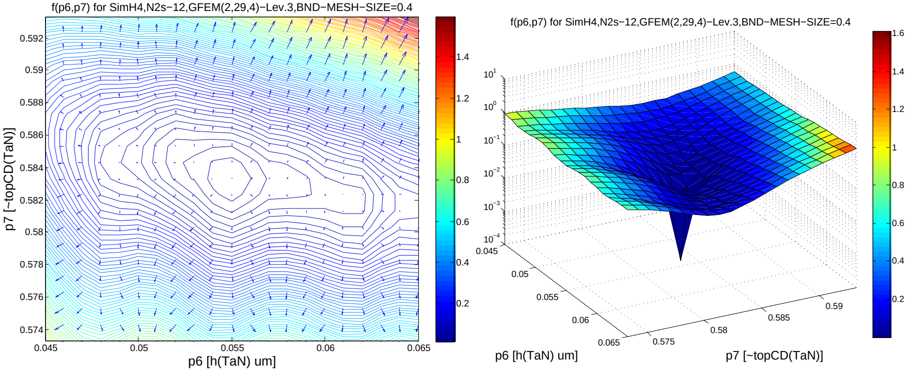
lev.	h_1	h_3	h_4	h_5	h_6	h_8
3	0.04719	0.26449	0.02184	0.73551	0.32085	0.27829
4	0.04939	0.27645	0.02276	0.73134	0.29526	0.26069
5	0.04988	0.27897	0.02295	0.73035	0.29177	0.25755
6	0.04997	0.27954	0.02299	0.73016	0.29099	0.25674
ex.v.	0.05000	0.27967	0.02300	0.73007	0.29068	0.25638


x 10^-3
deviation from the expected value
index of optimised parameter
1
2
3
4
5
6
8
x 10^-3
deviation from the expected value
index of optimised parameter



bad scaling and some facts ignored

f(p6,p7) for optimal 12 efficiencies, EUV mask



Outline

Tasks of sensitivity analysis:

- Theoretically: Huge amount of direct measurement data possible. Which part of this data is really needed for an accurate and fast reconstruction of the entities to be “measured” indirectly?
  $\Longrightarrow$ minimize the condition numbers of the mapping: $h \mapsto E(h)$
- Knowing the uncertainties of the direct measurement data, estimate the measurement uncertainties of the indirect measurement values!
- Estimate the uncertainties of the direct measurement data!
  $\Longrightarrow$ maximum likelihood estimator

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Conclusions

- Finite element method: good choice for the numerical solution of Maxwell's equations
- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Optimization of measurement data helpful
- Uncertainties of reconstructed parameters should be estimated

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Some references:

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Thank you for your attention!