A. Rathsfeld

$245^{th}$ 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"
1 Maxwell’s Equations and Rigorous Numerical Methods
   - Boundary Value Problems
   - Finite Element Method
   - Radiation Condition
   - Alternative Methods

2 Difficulties for Numerical Methods

3 Inverse Problems for Scatterometry
   - Full Inverse Problems
   - Finite Dimens. Operator Equation and Optimization Problem
   - Global Methods of Optimization
   - Gradient Based Methods

4 Sensitivity Analysis

5 Conclusions
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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. $E(x_1, x_2, x_3, t) = E(x_1, x_2, x_3)e^{-i\omega t}$)

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

- 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

\[
\Delta v(x_1, x_2) + k^2 v(x_1, x_2) = 0, \quad v = E_3, H_3
\]

- 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 $\nu$ to boundary face
  
  $\nu \times E = \nu \times E^{\text{incident}}$,  
  $\nu \times \nabla \times E = \nu \times \nabla \times E^{\text{incident}}$

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

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

- 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

\[
\int_{\Omega} \nabla \times E \cdot \nabla \times F - \int_{\Omega} k^2 E \cdot F + \int_{\Gamma} (TE) \cdot F = - \int_{\Gamma^+} E^{\text{incident}} \cdot F,
\]
for all \( F \) in \( H(\text{curl}, \Omega) \)

\[
a(E, F') = b(F'), \quad \text{for all } F \text{ in } H(\text{curl}, \Omega)
\]

with: \( T \) operator of boundary condition
\( \Omega \) 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 $\Omega = \bigcup_{j=1}^{J} \Omega_j$ with $\text{diam} \Omega_j \leq h$

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

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

$$a(E_h, F_h) = b(F_h), \quad \text{for all } F_h \text{ in } \mathcal{F}_h(\Omega)$$
choose a natural finite element basis $(\varphi_{h,m})$ in $\mathcal{F}_h(\Omega)$, FEM system is equivalent to matrix equation

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

$$M(\xi_m) = (\eta_m), \quad M = \left( a(\varphi_{h,m}, \varphi_{h,m'}) \right)_{m,m'}$$
For **Helmholtz** equation, piecewise linear nodal basis over hexagonal two-dimensional mesh: hat function

\[ \varphi_{h,m} \]

For **Curl-Curl** equation, edge elements (Nédélec):
- noncontinuous piecewise linear (polynomial) functions
- better approximation of \( \{ E : \nabla \times \nabla \times E = 0 \} \)

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\begin{align*}
\phi_{h,m}
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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)

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

- Radiation condition for outer domain different from full or half space (Hohage, Schmidt, Zschiedrich)
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?
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Full Inverse Problem:

- **Given:** the diffraction properties of structure (e.g. efficiencies $E_{j,l}^±$)
- **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


- avoid full inverse problems by using more a priori information on the structure: seek grating in class defined by a few parameters $h = (h_j)_{j=1}^J$ (parameter identification)
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- avoid full inverse problems by using more a priori information on the structure: seek grating in class defined by a few parameters $h = (h_j)_{j=1}^J$ (parameter identification)
given and reconstructed refractive index over cross section of grating
\[ h_i := p_i, \quad i = 1, 4, \quad h_i := \frac{p_i}{\text{period}}, \quad i = 2, 5, 7, \quad h_i := \frac{p_i}{p_{i-1}} , \quad i = 3, 6, 8 \]
Operator Equation:
measured data, efficiencies or phase shifts: \( E^{meas} = (E^m_{meas})_{m \in \mathcal{M}} \)
comp.data corresponding to parameters \( h \): \( E(h) = (E_m(h))_{m \in \mathcal{M}} \)
constraints: \( h_j^{min} \leq h_j \leq h_j^{max} \)

Optimization Problem:
minimize objective functional
\[
\Phi \left( E_m(h) \right) \rightarrow \text{inf}
\]
\[
\Phi \left( E_m(h) \right) := \sum_{m \in \mathcal{M}} \omega_m |E_m(h) - E^meas|^2
\]
box constraints: \( h_j^{min} \leq h_j \leq h_j^{max} \)
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$$E(h) = E^{meas}$$

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$$\Phi\left(E_m(h)\right) \longrightarrow \inf$$

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box constraints: $h_{j}^{min} \leq h_j \leq h_{j}^{max}$
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 $\Delta h$ the optimal solution of convex quadratic optimization problem with box constraints:

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

\[
\Phi\left(E_m(h)\right) := \sum_{m \in M} \omega_m |E_m(h) - E_{meas}^m|^2
\]

\[
\omega_m \sim \frac{1}{u(E_{meas}^m)^2}
\]
\[ h_i := p_i, \ i = 1, 4, \quad h_i := \frac{p_i}{\text{period}}, \ i = 2, 5, 7, \quad h_i := \frac{p_i}{p_{i-1}}, \ i = 3, 6, 8 \]
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bad scaling and some facts ignored
f(p6, p7) for optimal 12 efficiencies, EUV mask
Sensitivity Analysis

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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? 
  \[ \Rightarrow \text{minimize the condition numbers of the mapping: } h \mapsto E(h) \]

▷ 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! 
  \[ \Rightarrow \text{maximum likelihood estimator} \]
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- Reconstruction of geometric parameters possible (beyond diffraction limit)
- Optimization of measurement data helpful
- Uncertainties of reconstructed parameters should be estimated
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Acknowledgment

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Thank you for your attention!