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The concept of bidirectional operators and its application to the modeling of microstructures

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Geometric and diffractive branch of physical optics

The geometric Fourier transform

Physical and Geometrical Optics: Traditional Understanding



Physical and Geometrical Optics: Traditional Understanding



- Physical optics:
 - Light represented by electromagnetic fields which
 - are governed by Maxwell's equations.

- Geometrical/ray optics:
 - Light is represented by mathematical rays (with energy flux) which
 - are governed by Fremat's principle which is mathematically expressed by ray equation.

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Field Tracing Diagram: Free-Space Propagation





Example Spherical Field with Stop



Results of Fourier Transform

$$V_{\ell}(\boldsymbol{\rho}, z, \omega) = |V_{\ell}(\boldsymbol{\rho}, z, \omega)| \exp(\mathrm{i}\varphi_{\ell}(\boldsymbol{\rho}, z, \omega)) \left(\exp(\mathrm{i}\psi(\boldsymbol{\rho}, z, \omega))\right)$$

Decreasing radius of cruvature; increasing NA



Results of Fourier Transform



General Example with Aberrations



Field Zones by Mathematical Definition

• Geometric Fourier transform valid in specified modeling accuracy

• Field on reference plane is in **geometric field zone**

• Rigorous Fourier transform required in specified modeling accuracy

• Field on reference plane is in diffractive field zone



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- Physical optics:
 - Light represented by electromagnetic fields which
 - are governed by Maxwell's equations
 - Transition between diffractive/geometric branch fully specified and controlled by mathematical concept of geometric FT.

Physical optics in geometric zones is at least as fast as ray tracing!





• VirtualLab Fusion manages the transition between diffractive and geometric branches of physical optics automatically (steady development).

Non-sequential coupling of regional Maxwell Solver

Introduction of bidirectional operators

Physical-Optics System Modeling: Regional Maxwell Solver



Physical-Optics System Modeling: Regional Maxwell Solver



Sequential Connection of Regional Maxwell Solver



Non-Sequential Connection of Regional Maxwell Solver



In Fast Physical Optics we comply with the following strategies:

- 1. Tearing: The optical system is decomposed into various regions in which different types of specialized Maxwell solvers are applied.
- 2. Interconnection: The solutions per region are connected through non-sequential field tracing to solve Maxwell's equations in the entire system.

Non-Sequential Optical Field Tracing

Michael Kuhn, Frank Wyrowski, and Christian Hellmann

Kuhn, M.; Wyrowski, F. & Hellmann, C. (2012), Nonsequential optical field tracing, *in* T. Apel & O. Steinbach, ed., 'Finite Element Methods and Applications', Springer-Verlag, Berlin, , pp. 257-274.

Non-sequential Field Tracing

- Lightpaths through system are investigated
- Each lightpath is evaluated by field tracing



Field Tracing Diagrams: Examples



Field Tracing Operators: Space- and k-Domain

• The free-space operator equation is given by

$$E_{\perp}^{\text{out}}(\boldsymbol{\rho},\omega) = \mathcal{P}E_{\perp}^{\text{in}}(\boldsymbol{\rho},\omega)$$

and in matrix form by

$$\begin{pmatrix} E_x^{\text{out}}(\boldsymbol{\rho},\omega)\\ E_y^{\text{out}}(\boldsymbol{\rho},\omega) \end{pmatrix} = \begin{pmatrix} \mathcal{P} & 0\\ 0 & \mathcal{P} \end{pmatrix} \begin{pmatrix} E_x^{\text{in}}(\boldsymbol{\rho},\omega)\\ E_y^{\text{in}}(\boldsymbol{\rho},\omega) \end{pmatrix} \,.$$

• Analogously we have for the *B*-operator

$$E_{\perp}^{\text{out}}(\boldsymbol{\rho},\omega) = \mathcal{B}E_{\perp}^{\text{in}}(\boldsymbol{\rho},\omega)$$

and in matrix form

$$\begin{pmatrix} E_x^{\text{out}}(\boldsymbol{\rho},\omega) \\ E_y^{\text{out}}(\boldsymbol{\rho},\omega) \end{pmatrix} = \begin{pmatrix} \mathcal{B}_{xx} & \mathcal{B}_{xy} \\ \mathcal{B}_{yx} & \mathcal{B}_{yy} \end{pmatrix} \begin{pmatrix} E_x^{\text{in}}(\boldsymbol{\rho},\omega) \\ E_y^{\text{in}}(\boldsymbol{\rho},\omega) \end{pmatrix}.$$

• The free-space operator equation in *k*-domain is given by

$$ilde{E}^{ ext{out}}_{\perp}(\kappa,\omega) = ilde{\mathcal{P}} ilde{E}^{ ext{in}}_{\perp}(\kappa,\omega)$$

with $\kappa = (k_x, k_y)$. In matrix form we have

$$\begin{pmatrix} \tilde{E}_{\chi}^{\text{out}}(\boldsymbol{\kappa},\omega) \\ \tilde{E}_{y}^{\text{out}}(\boldsymbol{\kappa},\omega) \end{pmatrix} = \begin{pmatrix} \tilde{\mathcal{P}} & 0 \\ 0 & \tilde{\mathcal{P}} \end{pmatrix} \begin{pmatrix} \tilde{E}_{\chi}^{\text{in}}(\boldsymbol{\kappa},\omega) \\ \tilde{E}_{y}^{\text{in}}(\boldsymbol{\kappa},\omega) \end{pmatrix}$$

• Analogously we have for the *B*-operator

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Bidirectional Operator: k-Domain

• For the bidirectional operator in *k*-domain we have per matrix element the integral of the form

$$\tilde{V}^{\mathsf{out}}(k_x, k_y) = \int_{K^2} \tilde{B}(k_x, k_y, k'_x, k'_y) \tilde{V}^{\mathsf{in}}(k'_x, k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y \, .$$

with he integral kernel $\tilde{B}(k_x, k_y, k'_x, k'_y)$.

- Since $\tilde{V}^{in}(k'_x,k'_y)$ can be understood as a decomposition into (inhomogeneous) plane waves, the bidirectional operator provides the plane-waves response on one incident plane wave.
- The integral operator reduces to a multiplication for stratified media and gratings per order (with *k*-value mapping).



Bidirectional Operator: k-Domain

• For the bidirectional operator in *k*-domain trix element the integral of the form

Bidirectional operator Generalization of Bidirectional Scattering Distribution Function (BSDF).

$$\tilde{V}^{\text{out}}(k_x, k_y) = \int_{K^2} \tilde{B}(k_x, k_y, k'_x, k'_y) \tilde{V}^{\text{in}}(k'_x, k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y \, .$$

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Non-sequential coupling of regional Maxwell Solver

Coupling of FMM solver

Nonsequential Coupling of FMM Solvers



Theory Background

• Global S matrix



 Recursion with respect to number of regions / layers Non-sequential field tracing



 Recursion with respect to number of light paths

Planar Surface + Planar Surface

• Structure • Non-sequential field tracing



Rectangular Grating + Backside Coating

• Non-sequential field tracing



• ... with backside coating



<u>+1</u>

0

23.6%

18.1%

±1

0

0.762%

33.1%

Rectangular Grating + Backside Coating

• Non-sequential field tracing



... with backside coating



Rectangular + Sawtooth Grating (parallel)

• Non-sequential field tracing



• ... with sawtooth coating



Т	Eff.	R	Eff.
-1	28.1%	-1	0.65%
0	18.2%	0	0.923%
+1	51.4%	+1	0.74%
Rectangular + Sawtooth Grating (parallel)

• Non-sequential field tracing



... with sawtooth coating

550 nm



Computational Effort

• Parallel gratings



Global S matrix	Non-sequential field tracing
$\sim M^3$ (scaling with number of layers)	$\sim M^3$ (scaling with number of light paths)
with M as the number of diffraction (evanescent included) orders used in calculation	

• Crossed gratings



Global S matrix	Non-sequential field tracing
$ \sim (M_x \times M_y)^3 $ (scaling with number of layers)	$\sim (M_x^3 + M_y^3)$ (scaling with number of light paths)
with M_x and M_y as the number of diffraction (evanescent included) orders in both directions	

Rectangular + Sawtooth Grating (crossed)

- Structure
 - Front: rectangular grating (along *x* direction)
 - Back: sawtooth grating (along y direction)





Rectangular + Sawtooth Grating (crossed)

• Non-sequential field tracing (TM)





Rectangular + Sawtooth Grating (crossed)

Non-sequential field tracing (TE)





Rectangular + Sawtooth Grating (45° rotated)

- Structure
 - Front: rectangular grating (along *x* direction)
 - Back: sawtooth grating (along x-y diagonal direction)





Global S matrix (TM)

- ➔ No common period!
- → Huge computational effort even with approximated common period

Rectangular + Sawtooth Grating (45° rotated)



Х

T(1, 1)

T(0, 1)

• Non-sequential field tracing (TM)

Non-Sequential Connection of Regional Maxwell Solver



Curved Surfaces: Newton Rings



$$\widetilde{\mathcal{B}}_2 \xrightarrow{\widetilde{\mathcal{P}}} \widetilde{\mathcal{B}}_3$$

$$\tilde{V}^{\mathsf{out}}(k_x, k_y) = \int_{K^2} \tilde{B}(k_x, k_y, k'_x, k'_y) \tilde{V}^{\mathsf{in}}(k'_x, k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y$$

Curved Surfaces: Lenses and Freeform Surfaces



$$\rightarrow$$
 $\tilde{\mathcal{B}}_2 \xrightarrow{\tilde{\mathcal{P}}} \tilde{\mathcal{B}}_3$

$$\tilde{V}^{\mathsf{out}}(k_x, k_y) = \int_{K^2} \tilde{B}(k_x, k_y, k'_x, k'_y) \tilde{V}^{\mathsf{in}}(k'_x, k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y$$

B operator for curved surfaces

Local plane interface approach (LPIA)

Local Plane Interface Approximation (LPIA)



- For each k-value the bidirectional operator in space domain is the response of the surface on a plane wave.
- Response is obtained by local satisfaction of boundary condition.

$$\tilde{V}^{\mathsf{out}}(k_x,k_y) = \int_{K^2} \tilde{B}(k_x,k_y,k'_x,k'_y) \tilde{V}^{\mathsf{in}}(k'_x,k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y$$

Local Plane Interface Approximation (LPIA)



Local Plane Interface Approximation + Propagation



Local Plane Interface Approximation: B-Operator



Fourier transform of resulting field provides B-operator response for one incident k-value

$$\tilde{V}^{\mathsf{out}}(k_x, k_y) = \int_{K^2} \tilde{B}(k_x, k_y, k'_x, k'_y) \tilde{V}^{\mathsf{in}}(k'_x, k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y$$

Simulations: Specifications



Simulations: Fields Inside + On Surface



Simulations: Fields Inside + Propagated



Simulations: Transmitted Field On Surface (TE polarized)

High NA focus!





Field on interface: LPIA





Simulations: Transmitted Field On Surface (TE polarized)





Field inside



Field on interface: Comparison



Simulations: Transmitted Phase On Surface (TE polarized)



Field inside



Phase on interface: LPIA



Simulations: Transmitted Phase On Surface (TE polarized)



Field inside



Phase on interface: Comparison



Simulations: Transmitted Field Propagated (TE polarized)



Field inside



Field propagated: LPIA + Propagation



Simulations: Transmitted Field Propagated (TE polarized)



Field inside



Field propagated: Comparison



Simulations: Reflected Field On Surface (TE polarized)



Field inside



Field on interface: LPIA



Simulations: Reflected Field On Surface (TE polarized)





Field inside



Field on interface: Comparison



Simulations: Reflected Field Propagated (TE polarized)



Field inside



Field propagated: LPIA + Propagation



Simulations: Reflected Field Propagated (TE Propagation problem only! Can be solved. **Field inside** z20 µm n_1 Air n_2 Fused silica x0 100 µm **Field propagated: Rigoros Field propagated: Comparison** 2.5 0.8 \sim 0.6 S 0.4 **-**0.5 0.2 7 -0.03 -0.02 -0.04 0.01 0.02 0.03 -0.01 -0.02 0.02 -0.04 0 0.04 Coordinate [mm] Coordinate [mm]

0.04

Simulations: Reflected Field Propagated (TE polarized)



Simulations: Transmitted Field On Surface (TM polarized)



Field on interface: Rigorous





Field on interface: Comparison





Simulations: Specifications Changed



Simulations: Transmitted Field On Surface





Field inside



Field on interface: LPIA



Simulations: Transmitted Field On Surface





Field inside



Field on interface: Comparison



Simulations: Specifications Changed



Field inside



- Multiple scattering at surface is not taken into account by LPIA
- Observed for very high local NA
- LPIA algorithm can easily detect it!

Simulations: Specifications Changed



Simulations: Transmitted Field On Surface



Field inside



Field on interface: LPIA


Simulations: Transmitted Field On Surface



Field inside



Field on interface: Comparison



Simulations: Reflected Field On Surface



Field inside



Field on interface: LPIA



Simulations: Reflected Field On Surface



Field inside



Field on interface: Comparison



Simulations: Specifications Changed



Simulations: Transmitted Field On Surface



Field on interface: Rigoros



Field inside



Field on interface: LPIA



Simulations: Transmitted Field On Surface



Field on interface: Rigoros



Field inside



Field on interface: Comparison



Local Plane Interface Approximation (LPIA)



- Very reasonable technique for smooth surfaces.
- Multiple scattering at surface limits validity of LPIA.
- Can be easily detected by LPIA algorithm!
- No limitation of tickness but of local NA.
- Remark: Application of LPIA in geometric zones leads to fast B operators!

$$\tilde{V}^{\mathsf{out}}(k_x, k_y) = \int_{K^2} \tilde{B}(k_x, k_y, k'_x, k'_y) \tilde{V}^{\mathsf{in}}(k'_x, k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y$$

Discrete Height Steps: LPIA Identical with TEA



- For discrete height steps LPIA is identical with TEA.
- Diffraction/Scattering at edges WITHIN structure not taken into account
- Multiple scattering in structure not included.
- Vaildity: For thin profiles only (wavelength)
- Otherwise other methods, e.g. split-step (BPM, WPM, ...)

$$\tilde{V}^{\mathsf{out}}(k_x, k_y) = \int_{K^2} \tilde{B}(k_x, k_y, k'_x, k'_y) \tilde{V}^{\mathsf{in}}(k'_x, k'_y) \, \mathrm{d}k'_x \, \mathrm{d}k'_y$$



Structure Height Profile

Period = 50µm; Smallest Feature = 4.7410µm



Period = 20µm; Smallest Feature = 1.8964µm



Period = 10µm; Smallest Feature = 0.9482µm



Period = 5µm; Smallest Feature = 0.4741µm



Period = 50µm; Smallest Feature = 4.7410µm

Diffraction efficiencies



Period = 20µm; Smallest Feature = 1.8964µm



Period = 10µm; Smallest Feature = 0.9482µm



Period = 5µm; Smallest Feature = 0.4741µm



Summary

- Introduction of a geometric branch of physical optics with the help of the geometric Fourier transform.
- Fast physical optics enabled by non-sequential coupling of Maxwell solvers, which are mathematically expressed by B-operators.
- Generalization of BSDF concept in ray tracing.
- B-operators for curved surfaces by LPIA justified and limitation of validity can be detected by algorithm.
- B operator for thin stepped height profiles: TEA
- Thicker stepped profiles must be modeled by splitstep type techniques or rigorous approaches.

 Simulations done with VirtualLab Fusion software



 FEM with JCMSuite