Exact simulation of the diffraction of large, high-NA DOE-sections with O(NlogN) time and memory resort

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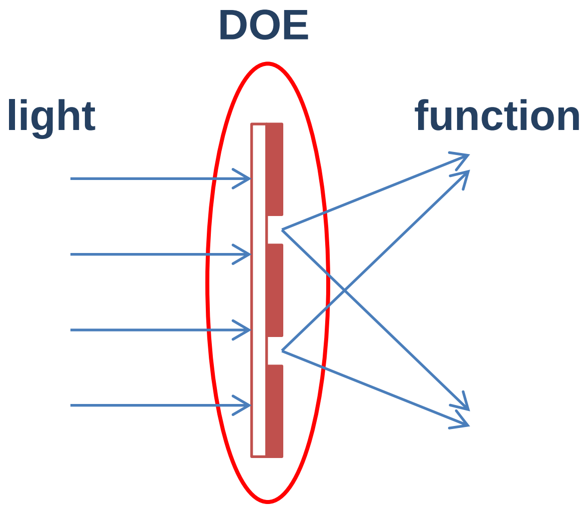
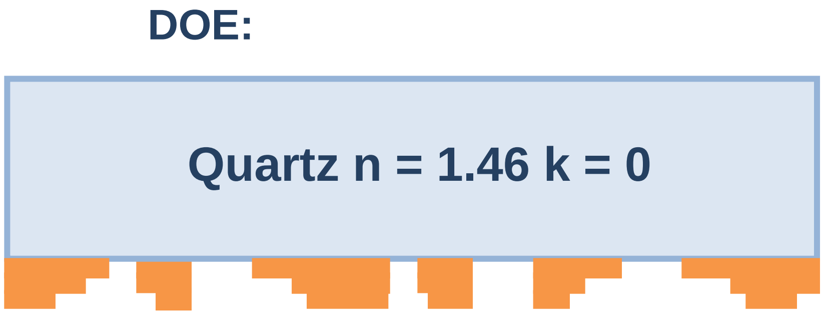
OUTLINE

- DOE simulation
- Generalized Source Method
- Three breakthroughs that make GSM ultrafast and memory sparing
- Numerical benchmarks
- Conclusions

DOE SIMULATION





n = 1.46 – 2.35 k < 0.01
Thickness < 1000 nm

Requirements on a new method for today's objectives in *DOE simulation*:

Rigorous

Fast and memory-sparing

Challenge:

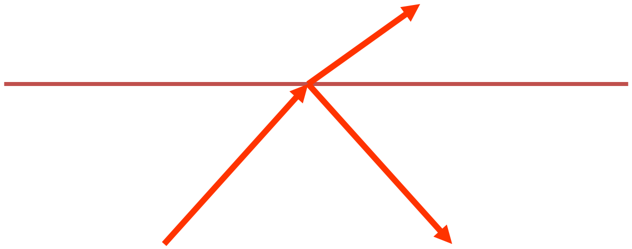
DOE reference method $\overset{?}{\equiv}$ DOE fast tool

Current exact methods (FDTD, FMM (RCWA)) are very far from this objective

TYPE OF APPROACH

A DOE is a planar structure

Plane waves are a basic solutions

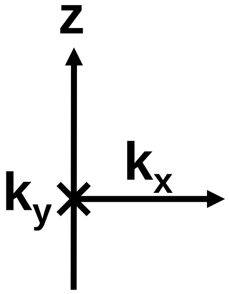


characterized by their in-plane wavevector projections k_x, k_y

An efficient resolution technique has to operate

 # in-plane in the reciprocal *k*-space k_x, k_y

 # in the direct space normally to the plane, along z



GENERALIZED SOURCE METHOD

The electromagnetic problem is characterized by the spatial permittivity distribution:

$$\varepsilon = \varepsilon(\mathbf{r})$$

1. Replace the initial problem with another one with $\varepsilon_b(\mathbf{r})$ which has an exact analytical solution for any source distribution:

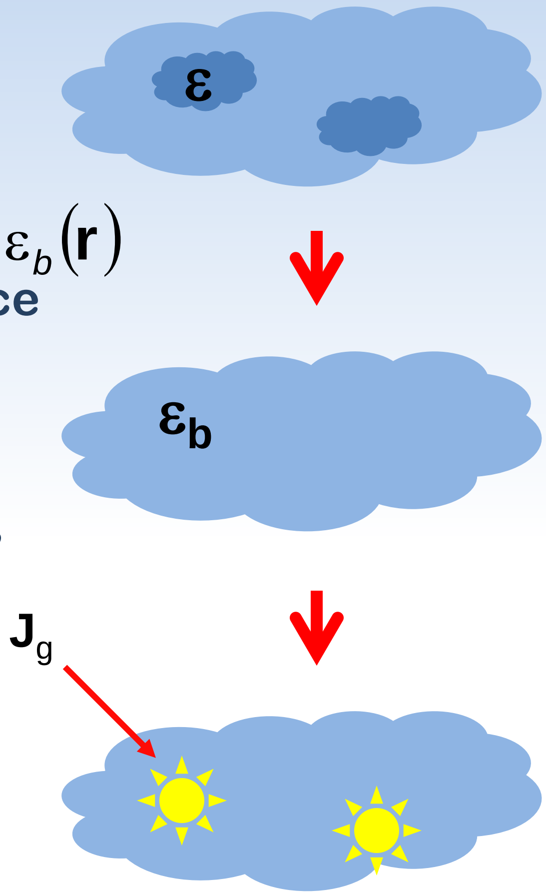
$$\nabla \times \nabla \times \mathbf{E} - \omega^2 \mu_0 \varepsilon_b(\mathbf{r}) \mathbf{E} = i\omega\mu_0 \mathbf{J} \quad \Rightarrow \quad \mathbf{E} = \aleph_b(\mathbf{J})$$

2. Take all nonzero differences between permittivities as generalized sources

$$\mathbf{J}_g = -i\omega(\varepsilon - \varepsilon_b)\mathbf{E}$$

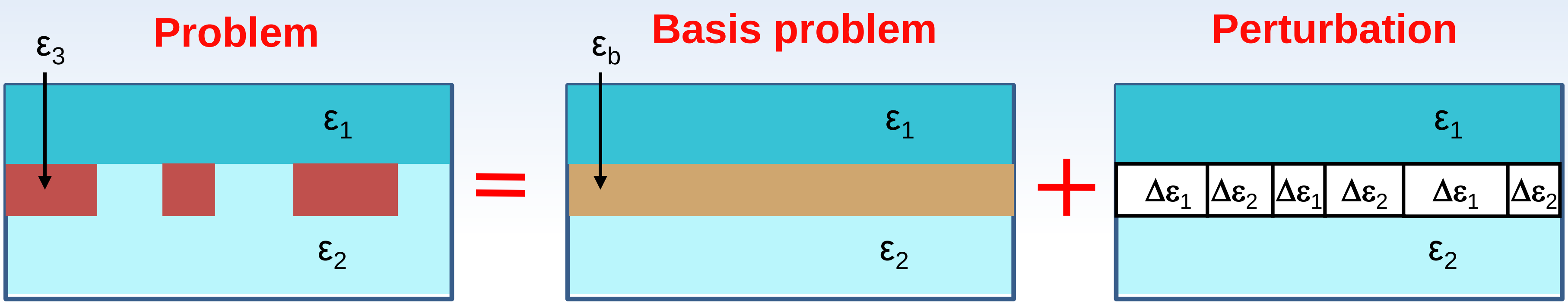
3. This leads to an implicit equation for unknown **E**

$$\mathbf{E} = \mathbf{E}_0 - \aleph_b\left[i\omega(\varepsilon - \varepsilon_b)\mathbf{E}\right]$$



[1]A.V. Tishchenko, Generalized source method: new possibilities for waveguide and grating problems // Opt. Quantum Electron., 32, 1971-1980 (2000)

Example of a binary corrugation



DOE pattern on substrate	**Homogeneous layer**	**Permittivity difference**
Solution unknown	***Complete solution known once for all***	***creates generalized sources:***

$$\mathbf{J}(x,y,z) = \mathbf{j}(z)\exp(ik_x x + ik_y y)$$

INTEGRAL EQUATION

Maxwell equations are reduced finally to the implicit integral equation:

$$\begin{pmatrix} a_n^{e\pm}(z) \\ a_n^{h\pm}(z) \end{pmatrix} = \delta_{n0} \begin{pmatrix} a_{inc}^{e\pm}(z) \\ a_{inc}^{h\pm}(z) \end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=-\infty}^{\infty} \sum_{\beta=x,y,z} \mathrm{P}_{n\alpha}^{\pm} \mathrm{R}_{n\alpha}^{\pm}(z,z') \mathrm{V}_{nm}^{\alpha\beta}(z') \left[\mathrm{Q}_{m\beta}^{+} \begin{pmatrix} a_m^{e+}(z') \\ a_m^{h+}(z') \end{pmatrix} + \mathrm{Q}_{m\beta}^{-} \begin{pmatrix} a_m^{e-}(z') \\ a_m^{h-}(z') \end{pmatrix} \right] \right\} dz'$$

INTEGRAL EQUATION

Integral equation:

$$\begin{pmatrix} a_n^{e\pm}(z) \\ a_n^{h\pm}(z) \end{pmatrix} = \delta_{n0} \begin{pmatrix} a_{inc}^{e\pm}(z) \\ a_{inc}^{h\pm}(z) \end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=-\infty}^{\infty} \sum_{\beta=x,y,z} \mathrm{P}_{n\alpha}^{\pm} \mathrm{R}_{n\alpha}^{\pm}(z,z') \mathrm{V}_{nm}^{\alpha\beta}(z') \left[\mathrm{Q}_{m\beta}^{+} \begin{pmatrix} a_m^{e+}(z') \\ a_m^{h+}(z') \end{pmatrix} + \mathrm{Q}_{m\beta}^{-} \begin{pmatrix} a_m^{e-}(z') \\ a_m^{h-}(z') \end{pmatrix} \right] \right\} dz'$$

Incident field harmonics

Integral equation:

$$\begin{pmatrix} a_n^{e\pm}(z) \\ a_n^{h\pm}(z) \end{pmatrix} = \delta_{n0} \begin{pmatrix} a_{inc}^{e\pm}(z) \\ a_{inc}^{h\pm}(z) \end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=-\infty}^{\infty} \sum_{\beta=x,y,z} \mathrm{P}_{n\alpha}^{\pm} \mathrm{R}_{n\alpha}^{\pm}(z,z') \mathrm{V}_{nm}^{\alpha\beta}(z') \left[\mathrm{Q}_{m\beta}^{+} \begin{pmatrix} a_m^{e+}(z') \\ a_m^{h+}(z') \end{pmatrix} + \mathrm{Q}_{m\beta}^{-} \begin{pmatrix} a_m^{e-}(z') \\ a_m^{h-}(z') \end{pmatrix} \right] \right\} dz'$$

Unknown amplitudes of TE- and TM-polarized harmonics

INTEGRAL EQUATION

Integral equation:

$$\begin{pmatrix} a_n^{e\pm}(z) \\ a_n^{h\pm}(z) \end{pmatrix} = \delta_{n0} \begin{pmatrix} a_{inc}^{e\pm}(z) \\ a_{inc}^{h\pm}(z) \end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=-\infty}^{\infty} \sum_{\beta=x,y,z} \mathrm{P}_{n\alpha}^{\pm} \mathrm{R}_{n\alpha}^{\pm}(z,z') \mathrm{V}_{nm}^{\alpha\beta}(z') \left[\mathrm{Q}_{m\beta}^{+} \begin{pmatrix} a_m^{e+}(z') \\ a_m^{h+}(z') \end{pmatrix} + \mathrm{Q}_{m\beta}^{-} \begin{pmatrix} a_m^{e-}(z') \\ a_m^{h-}(z') \end{pmatrix} \right] \right\} dz'$$

Transition matrix from TE- and TM-harmonics amplitudes to x-, y- and z-components of the electric field

$$\mathrm{Q}_n^{\pm} = \begin{pmatrix} \dfrac{k_{y0}}{\gamma_n} & \mp \dfrac{k_{xn} k_{zn}}{\omega \varepsilon_b \gamma_n} \\ -\dfrac{k_{xn}}{\gamma_n} & \mp \dfrac{k_{y0} k_{zn}}{\omega \varepsilon_b \gamma_n} \\ 0 & \dfrac{\gamma_n}{\omega \varepsilon_b} \end{pmatrix}$$

INTEGRAL EQUATION

Integral equation:

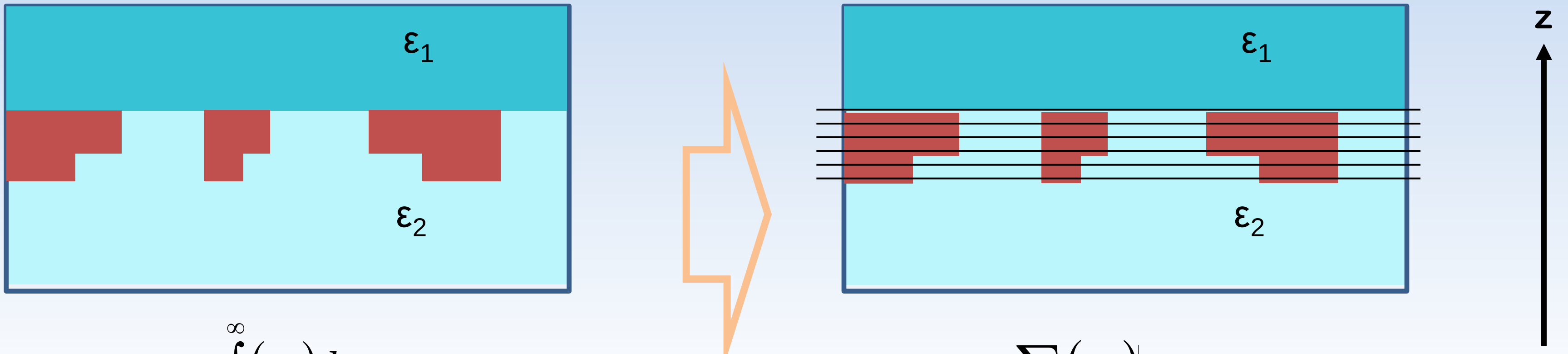
$$\begin{pmatrix} a_n^{e\pm}(z) \\ a_n^{h\pm}(z) \end{pmatrix} = \delta_{n0} \begin{pmatrix} a_{inc}^{e\pm}(z) \\ a_{inc}^{h\pm}(z) \end{pmatrix} + \sum_{\alpha=x,y,z} \int_{-\infty}^{\infty} \left\{ \sum_{m=-\infty}^{\infty} \sum_{\beta=x,y,z} \mathrm{P}_{n\alpha}^{\pm} \mathrm{R}_{n\alpha}^{\pm}(z,z') \mathrm{V}_{nm}^{\alpha\beta}(z') \left[\mathrm{Q}_{m\beta}^{+} \begin{pmatrix} a_m^{e+}(z') \\ a_m^{h+}(z') \end{pmatrix} + \mathrm{Q}_{m\beta}^{-} \begin{pmatrix} a_m^{e-}(z') \\ a_m^{h-}(z') \end{pmatrix} \right] \right\} dz'$$

Transition matrix from x-, y- and z-components of the electric field to TE- and TM-harmonics amplitudes

$$\mathrm{P}_n^{\pm} = \begin{pmatrix} -\dfrac{\omega\mu_0 k_{y0}}{2\gamma_n k_{zn}} & \dfrac{\omega\mu_0 k_{xn}}{2\gamma_n k_{zn}} & 0 \\ \pm\dfrac{k_{xn}}{2\gamma_n} & \pm\dfrac{k_{y0}}{2\gamma_n} & -\dfrac{\gamma_n}{2k_{zn}} \end{pmatrix}$$

LINEAR SYSTEM OF ALGEBRAIC EQUATIONS

Along z the integral is divided into slices:



$$\int_{-\infty}^{\infty}(\ldots)dz \quad \Rightarrow \quad \sum_p (\ldots)\Big|_{z=z_p}$$

The resulting equation is written in the form

$$\mathbf{a}_n^{\pm}(z_1,z_2)=\delta_{n0}\mathbf{a}_n^{inc\pm}(z_1,z_2)+\sum_{\alpha=x,y,z}\sum_{\beta=x,y,z}\mathrm{T}_{nq}^{\pm}\mathrm{P}_{n\alpha}^{\pm}\mathrm{V}_{nmq}^{\alpha\beta}\mathrm{Q}_{m\beta}^{\pm}\left(\mathrm{A}_{nmpq}^{\pm\pm}\right)^{-1}\delta_{m0}\mathbf{a}_{nq}^{inc\pm}(z_1,z_2)$$

Where the ***final matrix to be inverted*** is

$$\mathrm{A}_{nmpq}^{\pm\pm}=\mathrm{I}_{nmpq}^{\pm\pm}-\sum_{\alpha=x,y,z}\sum_{\beta=x,y,z}\mathrm{R}_{npq}^{\pm}\mathrm{P}_{n\alpha}^{\pm}\mathrm{V}_{nmq}^{\alpha\beta}\mathrm{Q}_{m\beta}^{\pm}$$

LINEAR SYSTEM OF ALGEBRAIC EQUATIONS

$$A^{\pm\pm}_{nmpq} = I^{\pm\pm}_{nmpq} - \sum_{\alpha=x,y,z}\sum_{\beta=x,y,z} R^{\pm}_{npq} P^{\pm}_{n\alpha} V^{\alpha\beta}_{nmq} Q^{\pm}_{m\beta}$$

Matrix containing exponential factors that describe the wave propagation along z-axis

$$R^{(e,h)(++)}_{npq} = \Delta h\left[\theta^{+}_{p-q} + \frac{r_n^{(L)e,h} r_n^{(U)e,h}\exp(2ik_{nz}h)}{1 - r_n^{(L)e,h} r_n^{(U)e,h}\exp(2ik_{nz}h)}\right]\exp[ik_{nz}\Delta h(p-q)]$$

$$R^{(e,h)(+-)}_{npq} = \Delta h\frac{r_n^{(L)e,h}\exp[ik_{nz}\Delta h(2N_L + 1 - p - q)]}{1 - r_n^{(L)e,h} r_n^{(U)e,h}\exp(2ik_{nz}h)}$$

$$R^{(e,h)(-+)}_{npq} = \Delta h\frac{r_n^{(U)e,h}\exp[ik_{nz}\Delta h(p + q - 1)]}{1 - r_n^{(L)e,h} r_n^{(U)e,h}\exp(2ik_{nz}h)}$$

$$R^{(e,h)(--)}_{npq} = \Delta h\left[\theta^{-}_{p-q} + \frac{r_n^{(L)e,h} r_n^{(U)e,h}\exp(2ik_{nz}h)}{1 - r_n^{(L)e,h} r_n^{(U)e,h}\exp(2ik_{nz}h)}\right]\exp[-ik_{nz}\Delta h(p-q)]$$

The 1st clue for ultra-fast computing:

Despite multiple reflections at interfaces matrix R keeps a Toeplitz structure

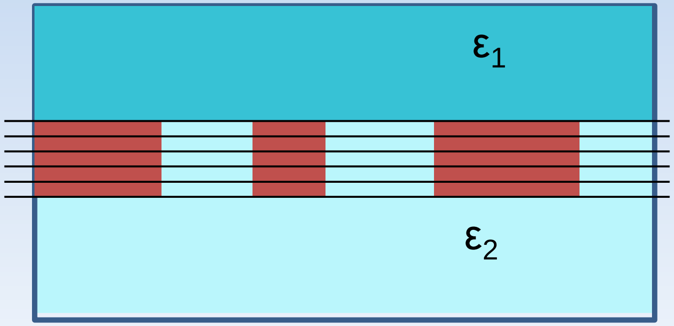
Fast numerical techniques applicable

DISCONTINUOUS PERMITTIVITY

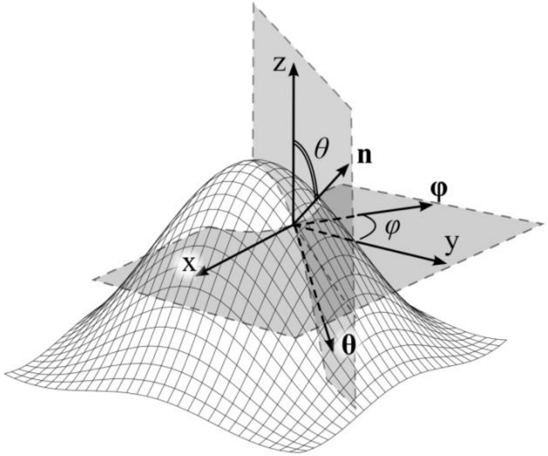
3D boundary conditions affect matrix multiplications

$$\mathbf{J} = -i\omega(\mathbf{D} - \mathbf{D}_b)$$

$$[\varepsilon]_{n-m}(E_{||})_m = (D_{||})_n \qquad (E_\perp)_n = \left[\frac{1}{\varepsilon}\right]_{n-m}(D_\perp)_m$$



FFT of 3D boundary condition functions



2nd clue for ultra-fast computing:

Matrix containing Fourier components of

 # permittivity

 # fields

 # local slope functions of boundaries

has Toeplitz structure

→ ***High accuracy achievable***

Last task: inversion of matrix A

$$A_{nmpq}^{\pm\pm} = I_{nmpq}^{\pm\pm} - \sum_{\alpha=x,y,z} \sum_{\beta=x,y,z} R_{npq}^{\pm} P_{n\alpha}^{\pm} V_{nmq}^{\alpha\beta} Q_{m\beta}^{\pm}$$

Assuming

***number of slices***:100

***number of diffraction orders*****: 100 and 100**

→ **size of matrix** A **is** $\sim 10^6$!!

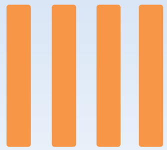
3rd clue for ultra-fast computing:

GMRES resolves a linear system in Krylov space in a few tens of iterative multiplications of a matrix by a vector

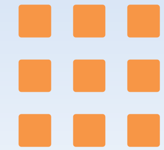
→ ***Fast and stable convergence attained***

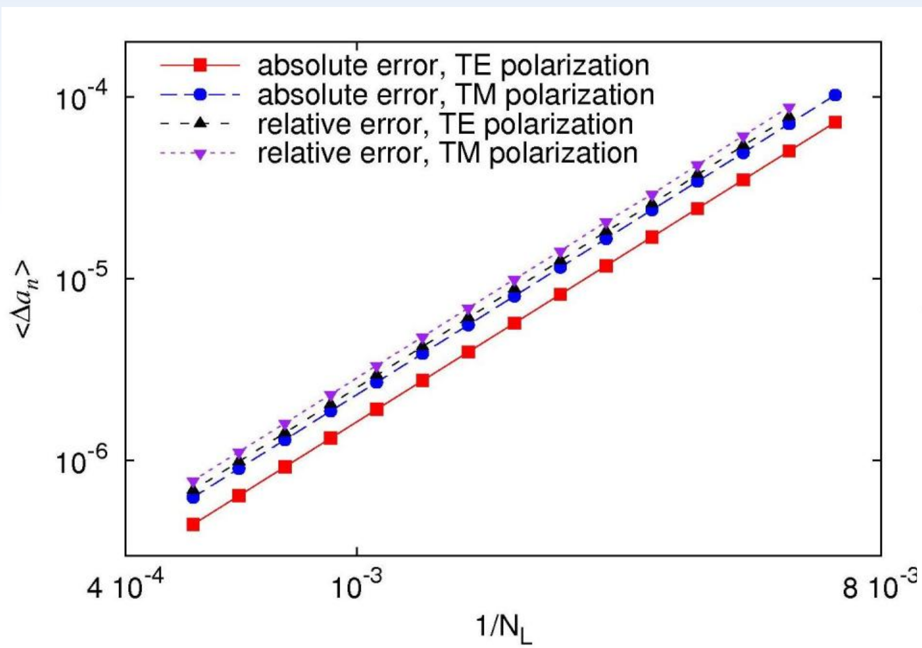
Comparison with Fourier-modal method (FMM, RCWA) versus number of slices N_L

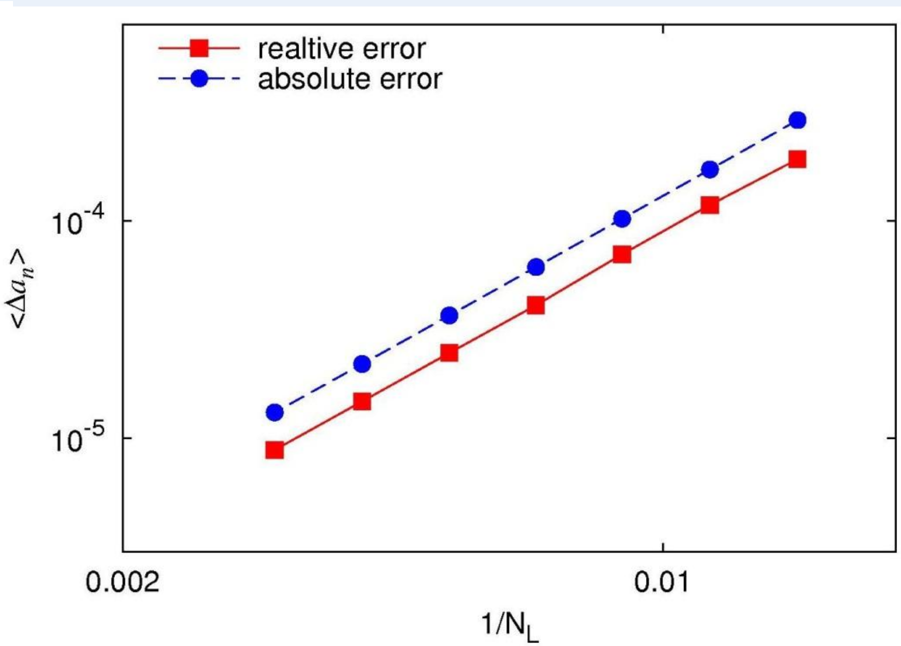
1D grating



2D grating



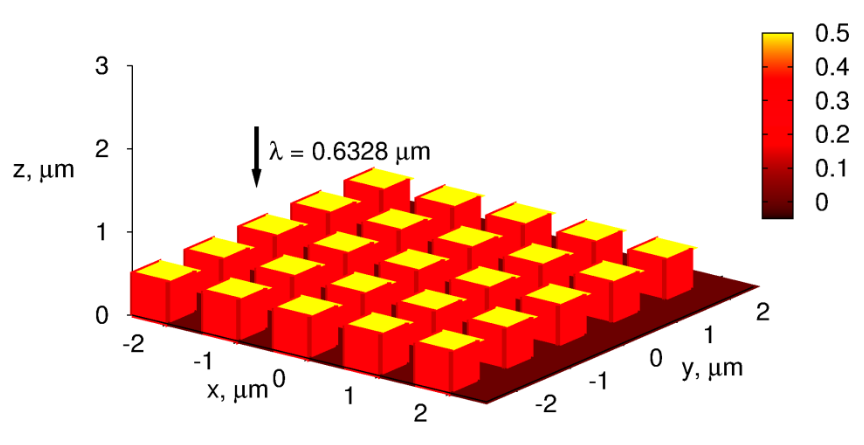




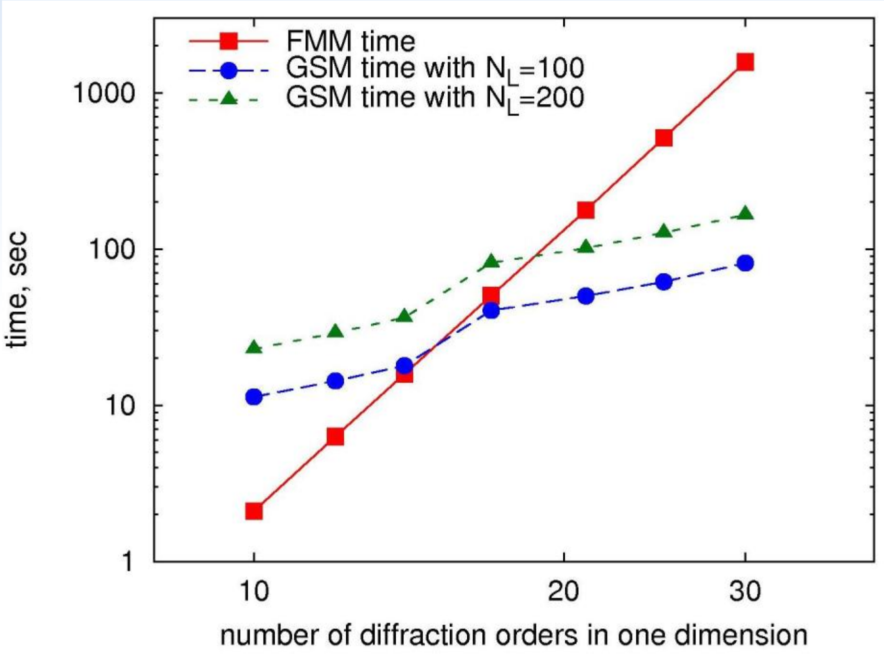
The dependencies resemble each other for different types of structures

NUMERICAL BENCHMARKS

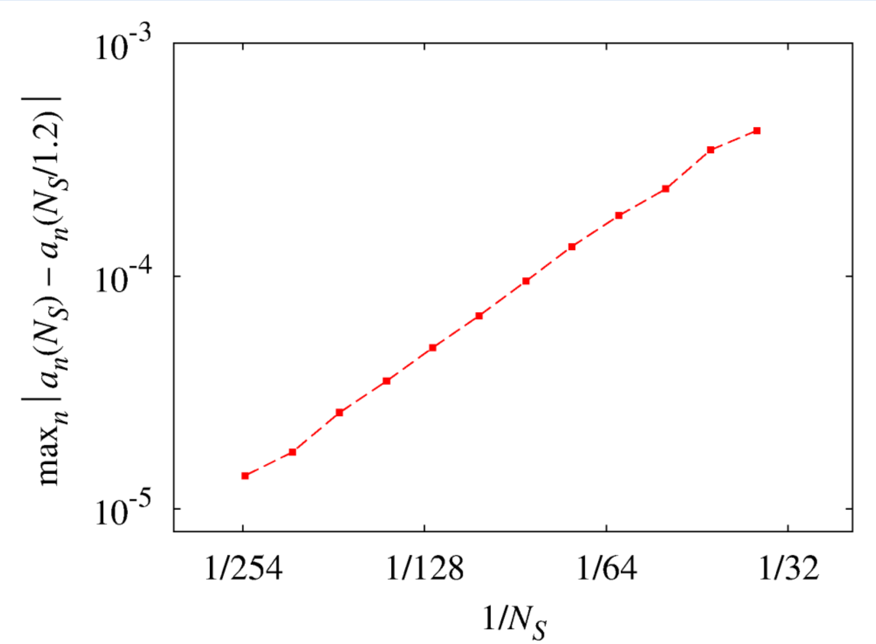
Comparison with Fourier-modal method (FMM, RCWA):

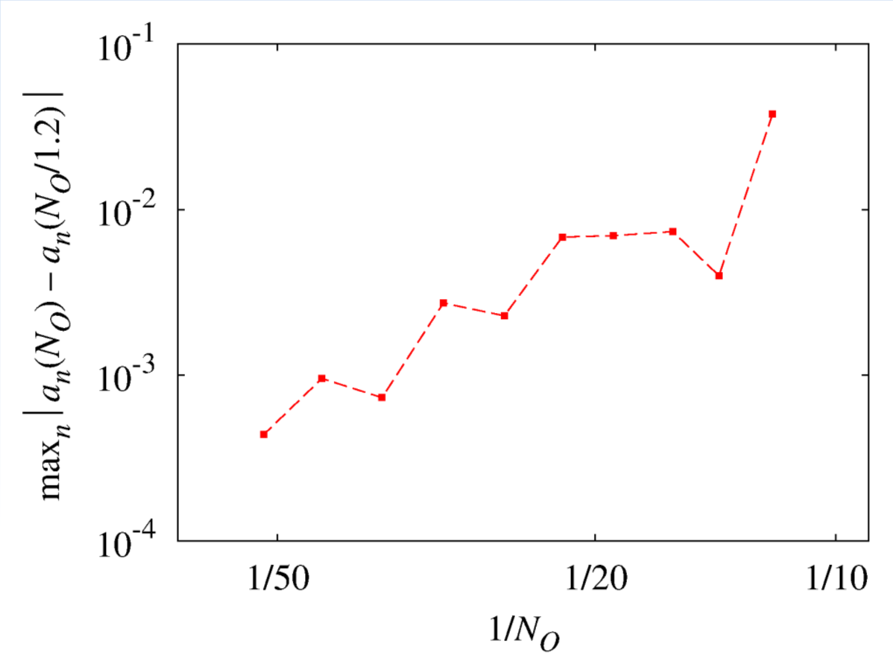


2D lamellar grating

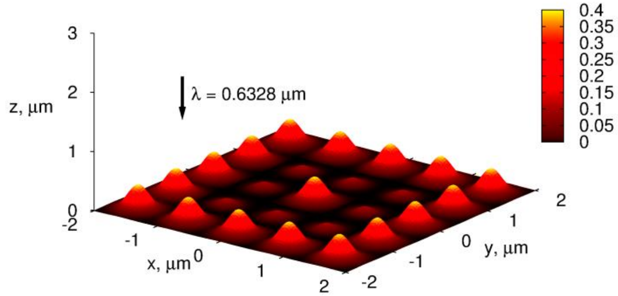


NUMERICAL BENCHMARKS



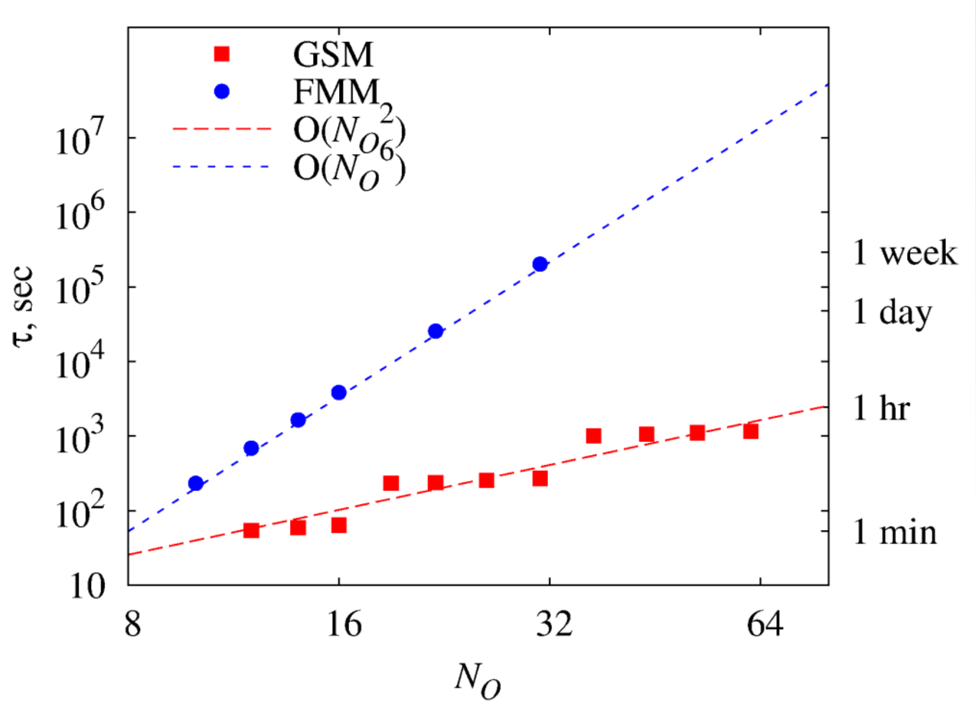


Convergence versus number of slices and diffraction orders

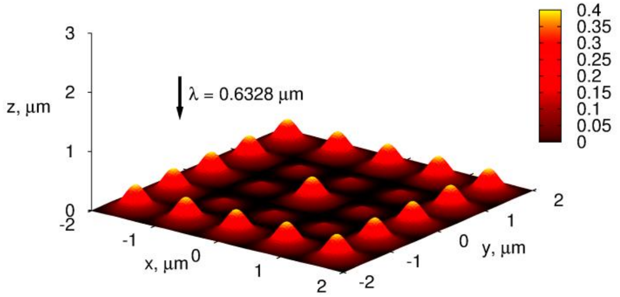


Period:	**4 μm**
Depth:	**0.4 μm**
Wavelength:	**0.633 μm**
DOE refractive index:	**2.1**
Cover refractive index:	**1.0**

NUMERICAL BENCHMARKS



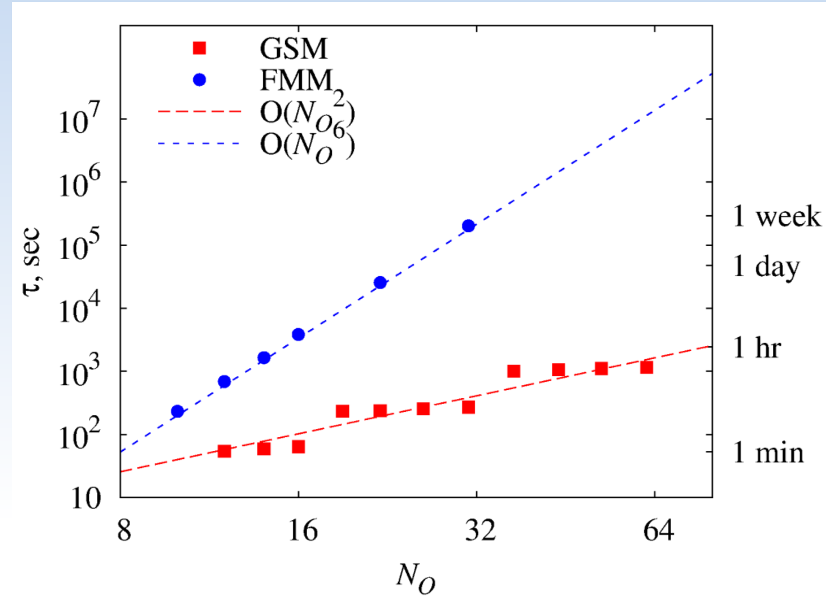
Processor 2.5 GHz
Memory 4 GB (Windows OS)

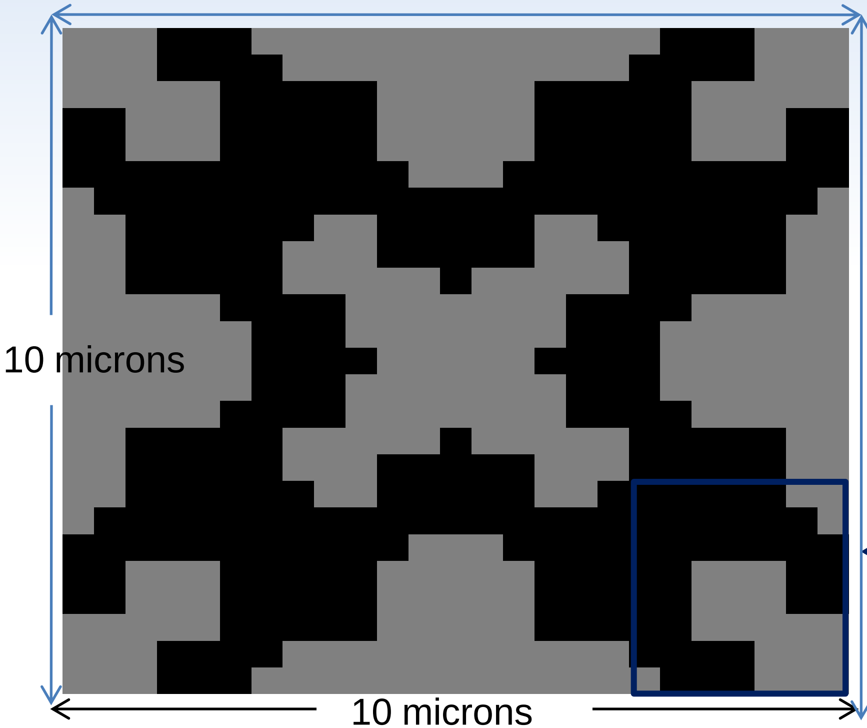


Period:	**4 μm**
Depth:	**0.4 μm**
Wavelength:	**0.6328 μm**
DOE refractive index:	**2.1**
Cover refractive index:	**1.0**

NUMERICAL BENCHMARKS

GSM needs 16 Gb of computer memory to calculate such DOE part with accuracy better than 10^{-3}





FMM fails to calculate more than this field because of memory limit

Parallel calculation by a GPU reduces 1 hour to 2-3 minutes!

CONCLUSION & PERSPECTIVES

- ✓ The GSM breaks through the time & memory limits of existing exact methods.
- ✓ The GSM permits exact modeling to invade the land occupied by scalar methods
- ✓ It makes it in three important application fields of diffraction/scattering:
  - Reticle and wafer latent image in advanced photolithography
  - Scattering layers for light extraction from (O)LEDs
  - Diffractive optics, e.g., high NA diffractive lenses

As from now on a big effort is needed to adapt and optimize the method to various application domain (*ref. Th. Kämpfe presentation in this conference*)

THANK YOU!