Fast and efficient modeling of metallic gratings diffraction with metric sources

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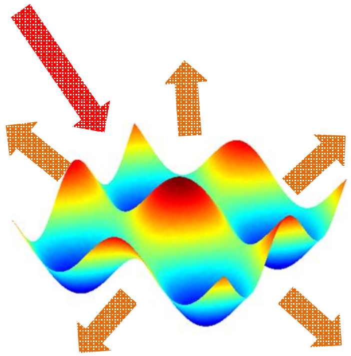
Outline

- Grating diffraction: Fourier space methods
- Curvilinear space
- Generalized Source Method (GSM)
- Generalized Metric Sources concept
- Method capabilities
- Conclusions



Linear diffraction on a periodic corrugation interface

Grating diffraction: Fourier space methods

Cartesian space:	Most suitable problems:
• Fourier-Modal Method (RCWA)	➢ dielectric, vertical walls or index gratings
• Differential Method	➢ dielectric complex shape gratings
• Generalized Source Method	➢ dielectric, complex shape gratings
Curvilinear space:	
• Chandezon Method	➢ metallic, smooth profile
• FMM with coordinate transform	➢ metallic, vertical walls

Grating diffraction: Fourier space methods

Cartesian space:

• Fourier-Modal Method (RCWA)	➢ $O(N^3)$
• Differential Method	➢ $O(N^3)$
• Generalized Source Method	➢ $O(N\log N)$

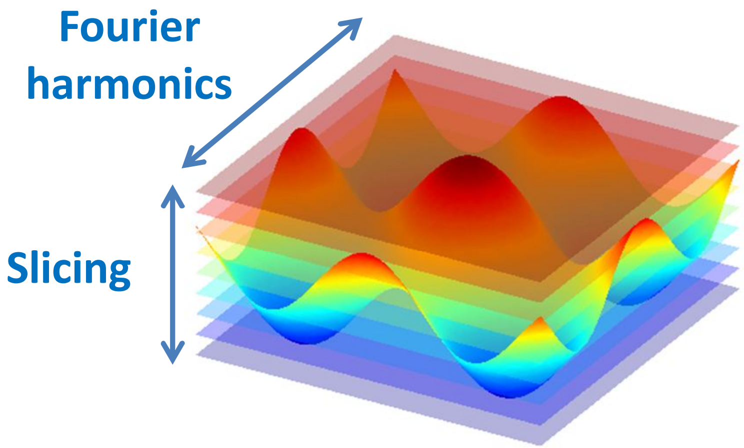
Curvilinear space:

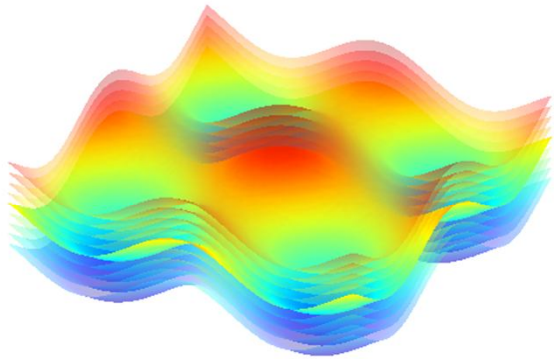
• Chandezon Method	➢ $O(N^3)$
• FMM with coordinate transform	➢ $O(N^3)$

O(NlogN) method for complex corrugated metallic gratings?

Curvilinear space

Periodic corrugation treatment:





GSM, FMM: slicing approximation in Cartesian coordinates

C-method: slicing approximation in curvilinear coordinates

- **only single-valued profile functions;**
- **similar transformation in the whole 2D/3D space.**

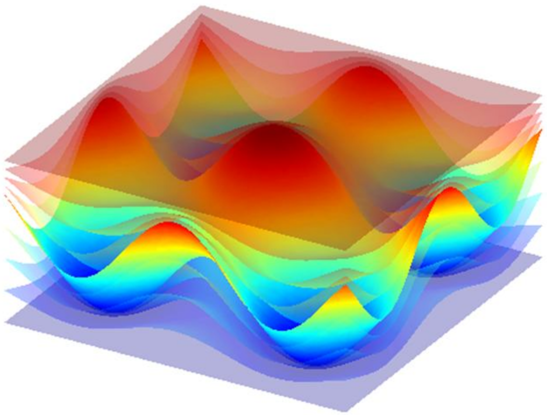
Curvilinear space

KEY IDEA: transform only in a bounded region

Cartesian space region →

Curvilinear space region →

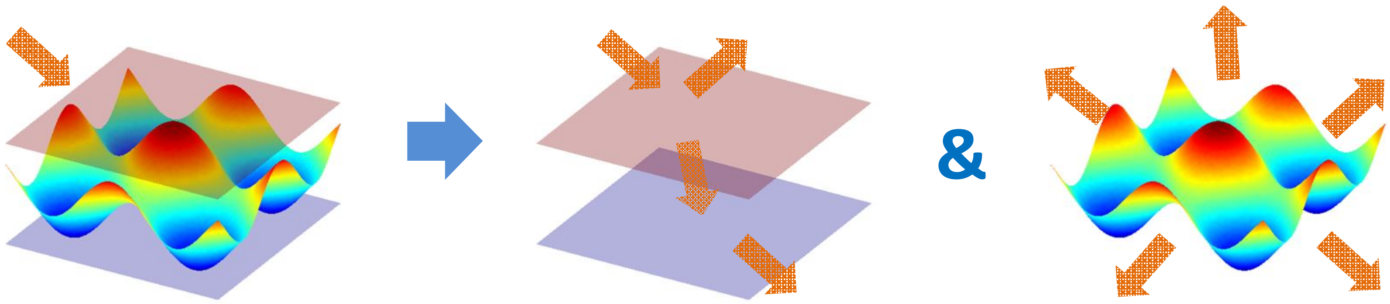
Cartesian space region →



Curvilinear coordinates continuously become Cartesian at interfaces of the grating region.

Slicing in curvilinear coordinates in a bounded region

Generalized Source Method



Diffraction or scattering problem	Basis medium + basis analytic solution	Difference between initial and basis media gives rise to the generalized sources
$\boldsymbol{\varepsilon(\vec{r})}$ $\nabla \times \vec{E} = i\omega\mu_0 \vec{H}$ $\nabla \times \vec{H} = \vec{J} - i\omega\varepsilon\vec{E}$	$\boldsymbol{\varepsilon_b(\vec{r})}$ $\nabla \times \vec{E} = i\omega\mu_0 \vec{H}$ $\nabla \times \vec{H} = -i\omega\varepsilon_b\vec{E}$	$\vec{J}_{gen} = -i\omega(\varepsilon - \varepsilon_b)\vec{E}$

- Implicit linear equation: $\vec{E} = \vec{E}_{inc} + \aleph\left(-i\omega(\varepsilon - \varepsilon_b)\vec{E}\right)$
- Discretization: Fourier space + Slicing
- GMRES+FFT assisted solution of the resulting algebraic system in O(NlogN) time and O(N) memory resort.

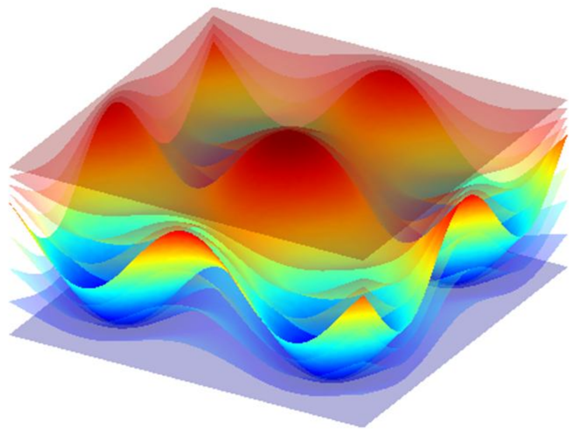
Generalized Metric Sources concept

Maxwell's equations

$$\nabla \times \vec{E} = -\vec{M} + i\omega\mu_0\vec{H}$$
$$\nabla \times \vec{H} = \vec{J} - i\omega\varepsilon\vec{E}$$

in a curvilinear space become

$$\xi^{\alpha\beta\gamma}\partial_\beta E_\gamma = -M^\alpha + i\omega\mu_0\sqrt{g}g^{\alpha\beta}H_\beta$$
$$\xi^{\alpha\beta\gamma}\partial_\beta H_\gamma = J^\alpha - i\omega\varepsilon\sqrt{g}g^{\alpha\beta}E_\beta$$



In accordance with the GSM rationale we split equations into a basis part

$$\xi^{\alpha\beta\gamma}\partial_\beta E_\gamma = i\omega\mu_0\delta^{\alpha\beta}H_\beta$$
$$\xi^{\alpha\beta\gamma}\partial_\beta H_\gamma = -i\omega\varepsilon_b\delta^{\alpha\beta}E_\beta$$

and Generalized Metric Sources

$$M^\alpha = -i\omega\mu_0\left(\sqrt{g}g^{\alpha\beta} - \delta^{\alpha\beta}\right)H_\beta$$
$$J^\alpha = -i\omega\varepsilon_b\left(\sqrt{g}g^{\alpha\beta} - \delta^{\alpha\beta}\right)E_\beta$$

Coordinate transformation in a grating region

$$q^i = q^i(x_1, x_2, x_3)$$

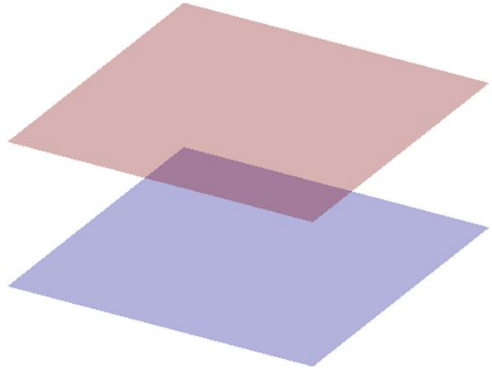
Fields are transformed via metric tensor:

$$g^{\alpha\beta} = \sum_\gamma \frac{\partial q^\alpha}{\partial x_\gamma}\frac{\partial q^\beta}{\partial x_\gamma},\ g = \det(g_{\alpha\beta})$$

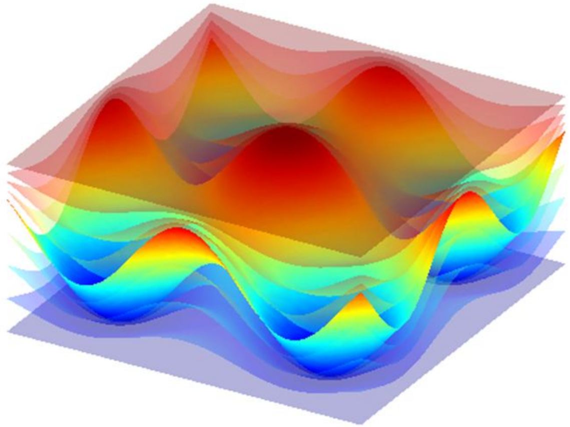
Generalized Metric Sources concept

Basis part:

$$\xi^{\alpha\beta\gamma}\partial_\beta E_\gamma = i\omega\mu_0\delta^{\alpha\beta}H_\beta, \qquad \nabla\times\vec{E} = i\omega\mu_0\vec{H}$$
$$\xi^{\alpha\beta\gamma}\partial_\beta H_\gamma = -i\omega\varepsilon_b\delta^{\alpha\beta}E_\beta. \leftrightarrow \nabla\times\vec{H} = -i\omega\varepsilon_b\vec{E}$$



is similar to the Maxwell's equations in Cartesian metric, and continuously become the Maxwell's equations at grating region boundaries

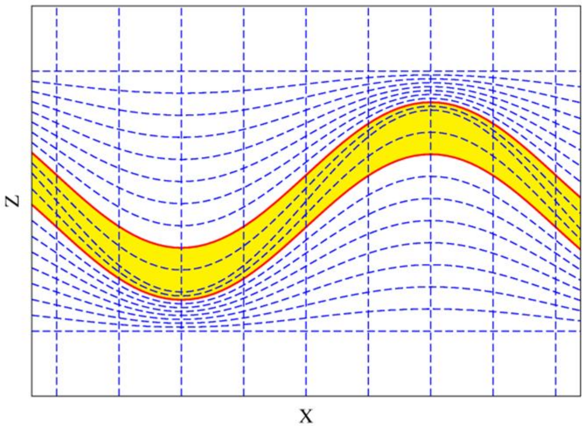


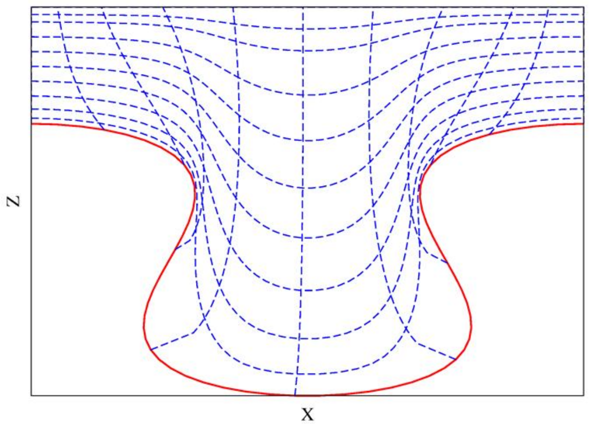
Generalized Metric Sources

$$M^\alpha = -i\omega\mu_0\left(\sqrt{g}g^{\alpha\beta} - \delta^{\alpha\beta}\right)H_\beta$$
$$J^\alpha = -i\omega\varepsilon_b\left(\sqrt{g}g^{\alpha\beta} - \delta^{\alpha\beta}\right)E_\beta$$

Method capabilities

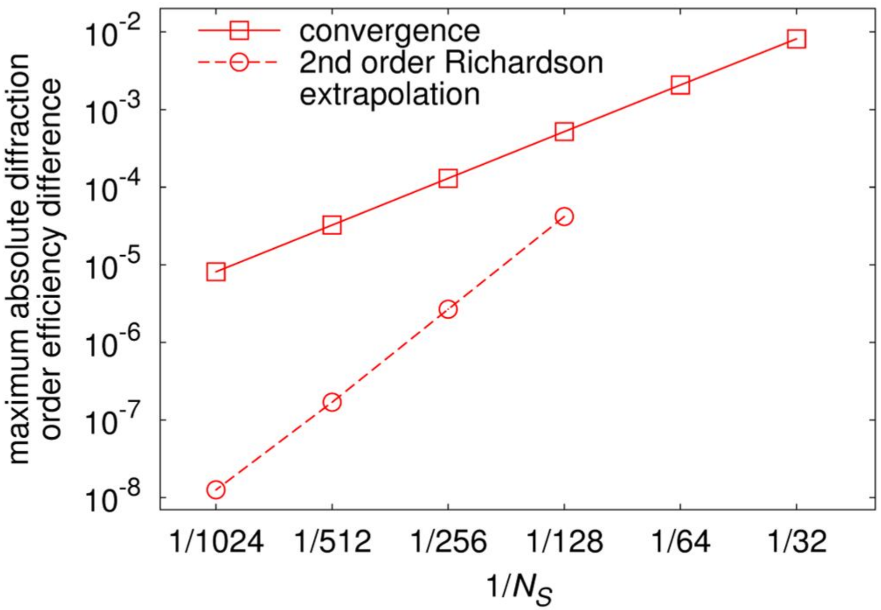
- ✓ Smooth profile gratings;
- ✓ Vertical wall gratings;
- ✓ “Overhanging” gratings;
- ✓ Multilayer periodic structures with different layer shapes;
- ✓ …

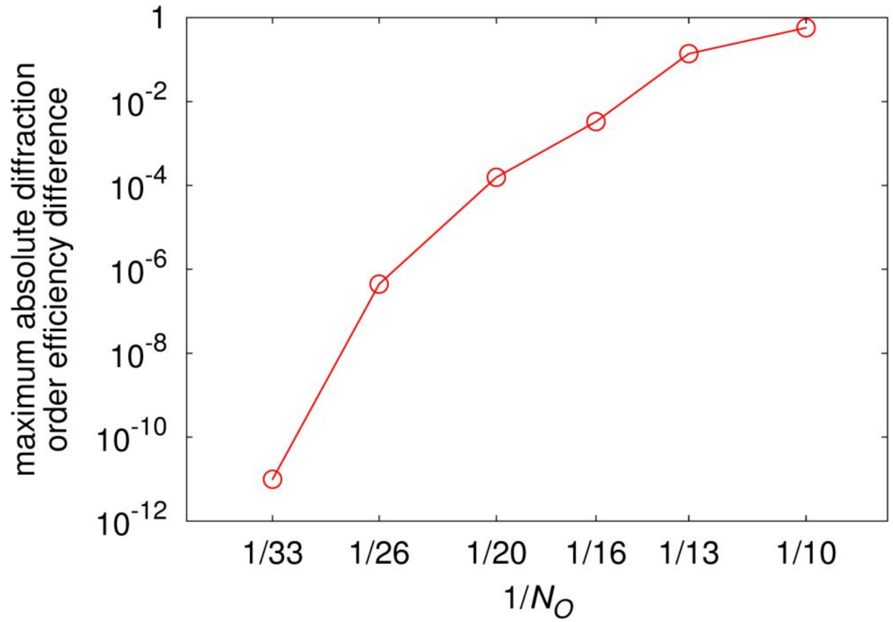




Method capabilities

Convergence example:

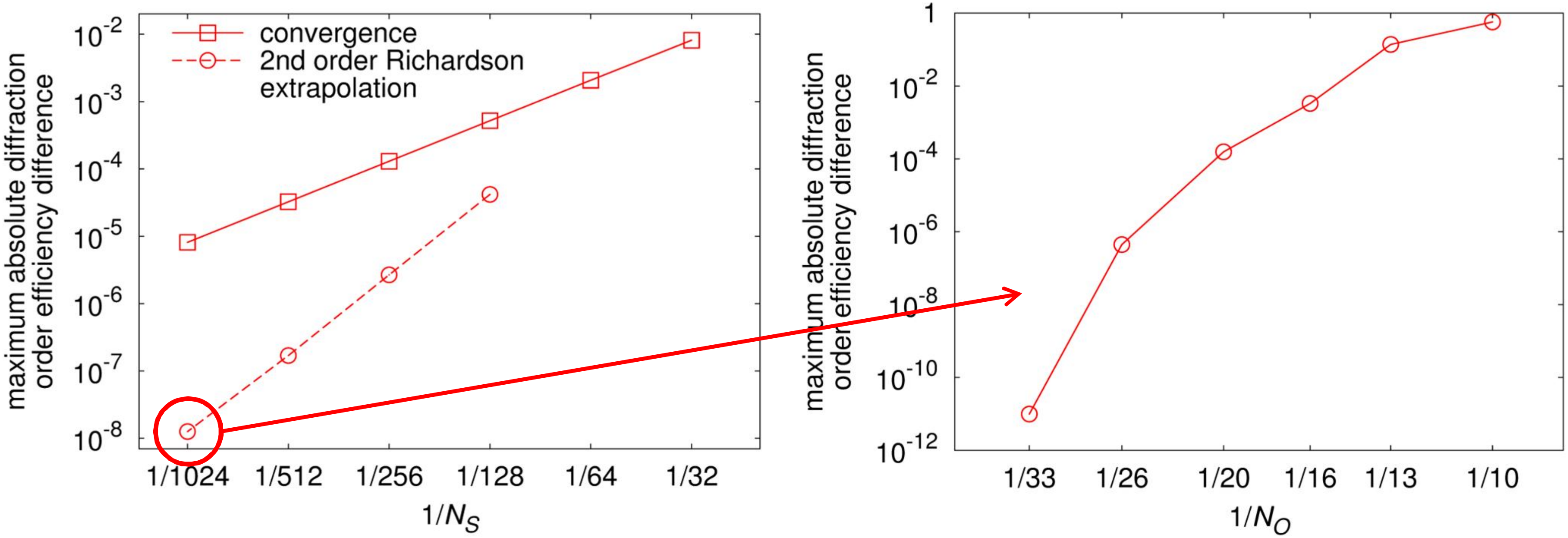




- **convergence is similar for both metallic and dielectric gratings;**
- **convergence over slice number is polynomial and can be significantly increased by use of the second order Richardson extrapolation;**
- **convergence over diffraction order number is obtained by taking the best solutions from the convergence over slice number.**

Method capabilities

Convergence example:



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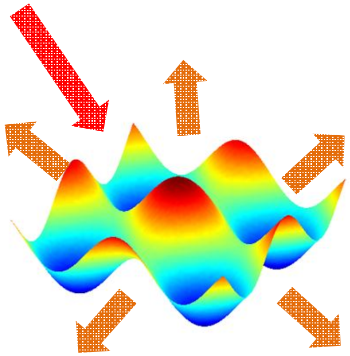
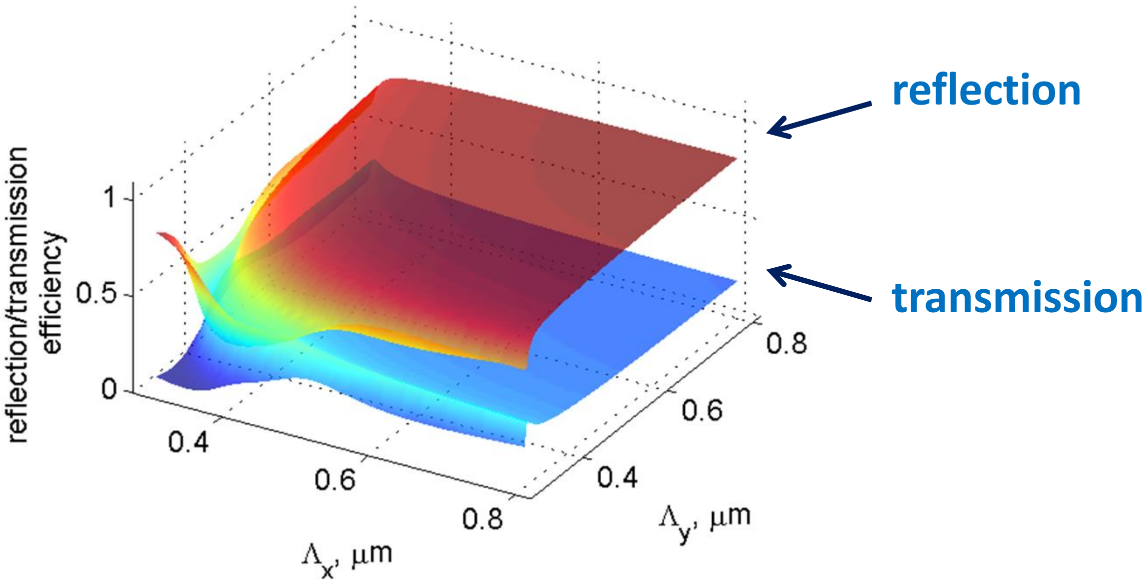
Method capabilities

2D sinusoidal grating abnormal transmission





0-th order reflection and transmission efficiencies depending on two grating periods for diffraction of a plane wave at wavelength 0.6328 µm under 10° incidence on a gold sinusoidal grating of depth 0.05 µm.

GSMCC for 1D gratings: A.A.Shcherbakov, A.V.Tishchenko. Efficient curvilinear coordinate method for grating diffraction simulation // Opt. Express. 21. No21. 25236-25247 (2013)

Conclusions

- ✓ Computationally and memory efficient (linear time complexity and memory requirements) volume integral curvilinear coordinate Fourier space method for grating diffraction simulation.
- ✓ Both metallic and dielectric gratings: similar convergence.
- ✓ High accuracy achievable
- ✓ No implicit use of the Rayleigh hypothesis: no restrictions for grating shapes and depths.
- ✓ Possible to use parallel GPU-enabled computations: about 50 times faster diffraction simulation.

Thank you

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The work was supported in part by the Russian Ministry of Education and Science (program 5Top100), and the Russian Foundation for Basic Research (grant # NK 14-07-31352\14)