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Numerical Simulation of Light Propagation Through Composite and Anisotropic Media Using Supercomputers

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Introduction

- The development of coherent sources of optical radiation, lasers, is often referred to as ”optical revolution”.
- Today we are witness to a new great progress in optical technologies connected with soft matter materials and optical metamaterials. It opens unique opportunities for dynamic control of light propagation.
- Numerical simulation is of great importance for better understanding of complex phenomena connected with light propagation through non-homogeneous, anisotropic and structured media as well as for development of new optical technologies.
- With the advent of modern supercomputers, numerical simulation of quite complicated optical systems and devices based on direct solving Maxwell’s equations has become feasible.
- In the present talk some examples of numerical simulations of problems connected with laser processing of materials, development of fiber-coupled liquid crystal systems and generation of ”optical vortices” using liquid crystals will be described.

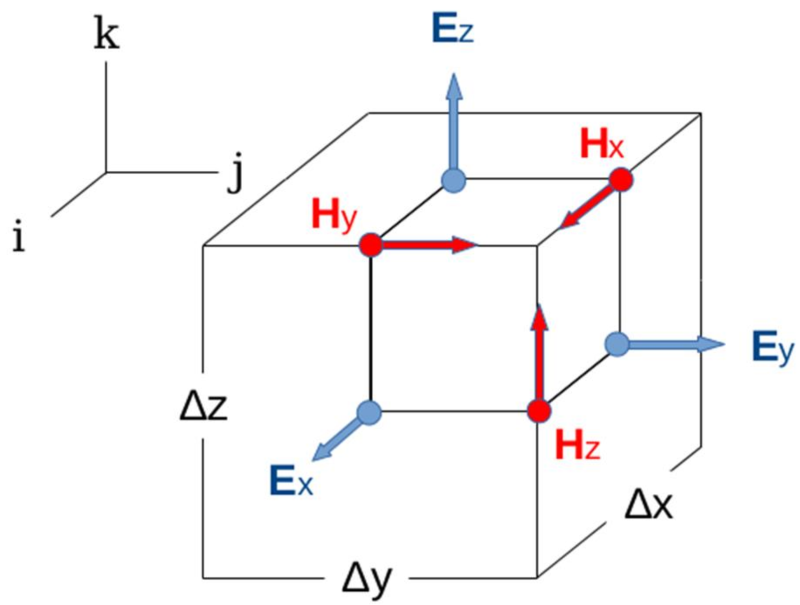
Maxwell's equations and FDTD numerical scheme

$$\frac{\partial \mathbf{D}}{\partial t} = -(\mathbf{J} + \sigma_e \mathbf{E}) + \nabla \times \mathbf{H}, \qquad \mathbf{D} = \bar{\bar{\epsilon}}\,\mathbf{E},$$

$$\frac{\partial \mathbf{B}}{\partial t} = -(\mathbf{M} + \sigma_m \mathbf{H}) - \nabla \times \mathbf{E}, \qquad \mathbf{B} = \bar{\bar{\mu}}\,\mathbf{H}.$$

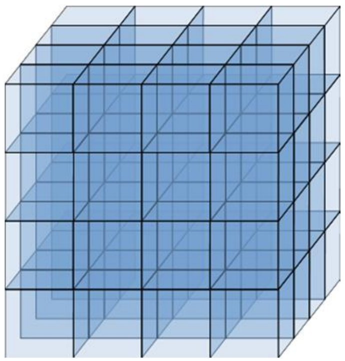
The FDTD (K.S. Yee, 1966) is a simple but smart devised and efficient second order numerical scheme using a grid staggered both in space and time.

To avoid false numerical reflections of scattered waves from boundaries of the computational domain, the uniaxial PML (Berenger, 1996) technique is employed.

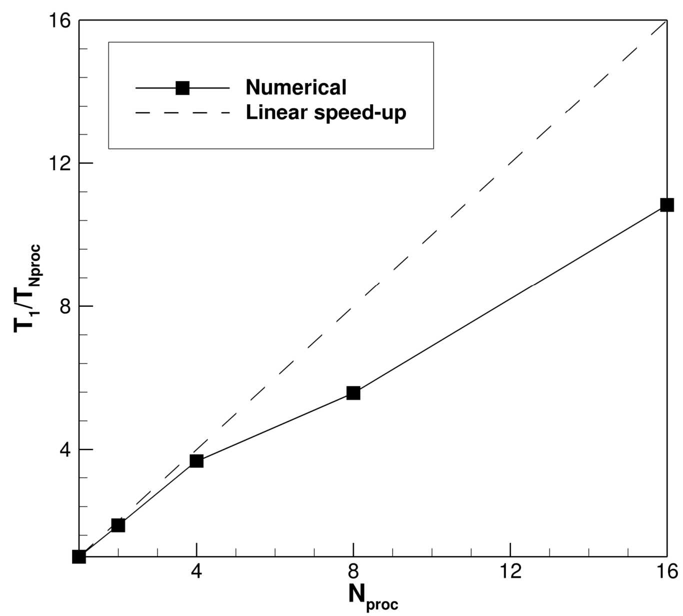


Numerical Implementation

- The code in Fortran-90 is parallelized using MPI.
- In different simulations presented below the spatial resolution is from 10 up to 30 grid cells per a wavelength.
- The computational domain is divided into rectangular blocks and each block is assigned to one computational core. Typically, the block consists of $150^3 = 3.375 \cdot 10^6$ cells.
- The largest grid used contained $6 \cdot 10^8$ cells, 180 cores were used to perform numerical simulations on this grid.
- The efficiency of parallelization was close to 70%

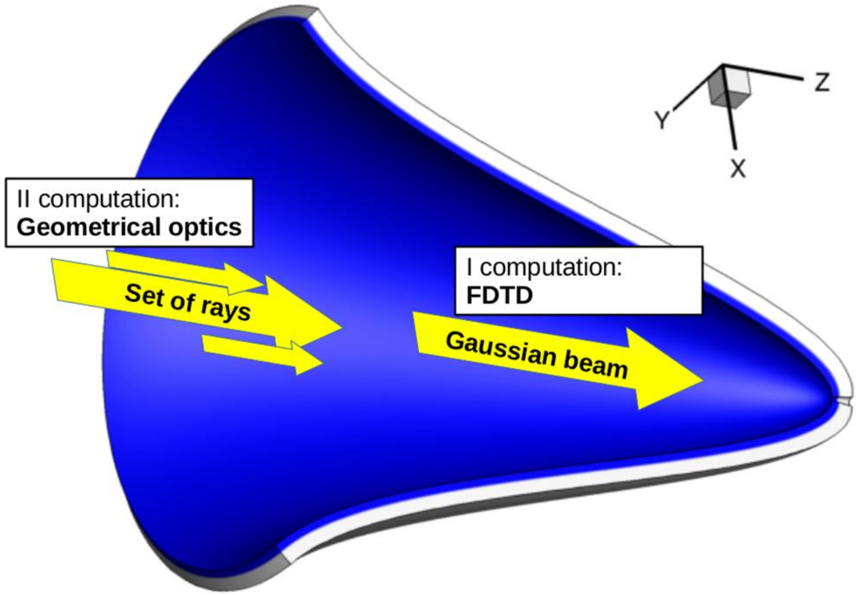


Geometrical domain decomposition



Numerical speed-up

Laser Drilling, I

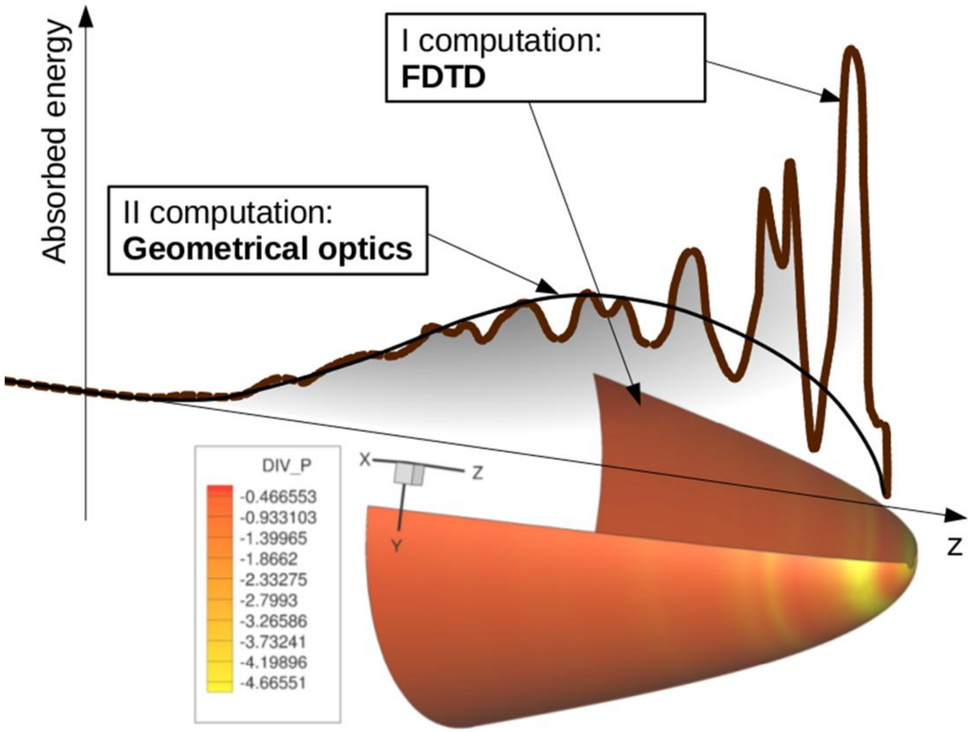


Schematic of laser drilling problem

- A Gaussian beam of circularly polarized laser radiation interacts with a cavity in a metal model.
- The aim is to calculate the absorbed power distribution in the model.
- Usually this problem is solved with geometrical optics by tracing propagation, reflection and refraction of light rays.
- However, in many cases it is not correct because small

features of the treated surface can be comparable in size with the radiation wavelength. So, it is preferable to use wave optics and solve Maxwell's equations.

Laser Drilling, II

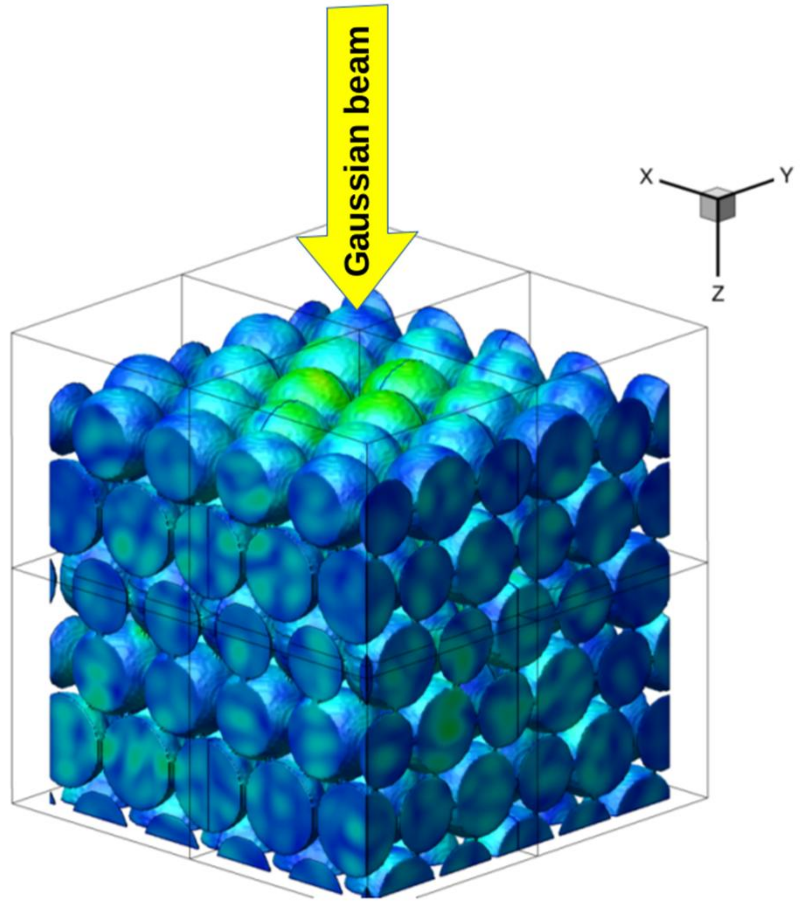


The surface distribution of time-averaged value of the Poynting vector divergence and its distribution along the axis

- There is a substantial qualitative difference of results obtained with wave and geometrical optics.
- The results of FDTD simulations point out that one possible reason for deterioration of laser drilling quality is an annular corrugation of the cavity bottom.

Laser Melting and Sintering, I

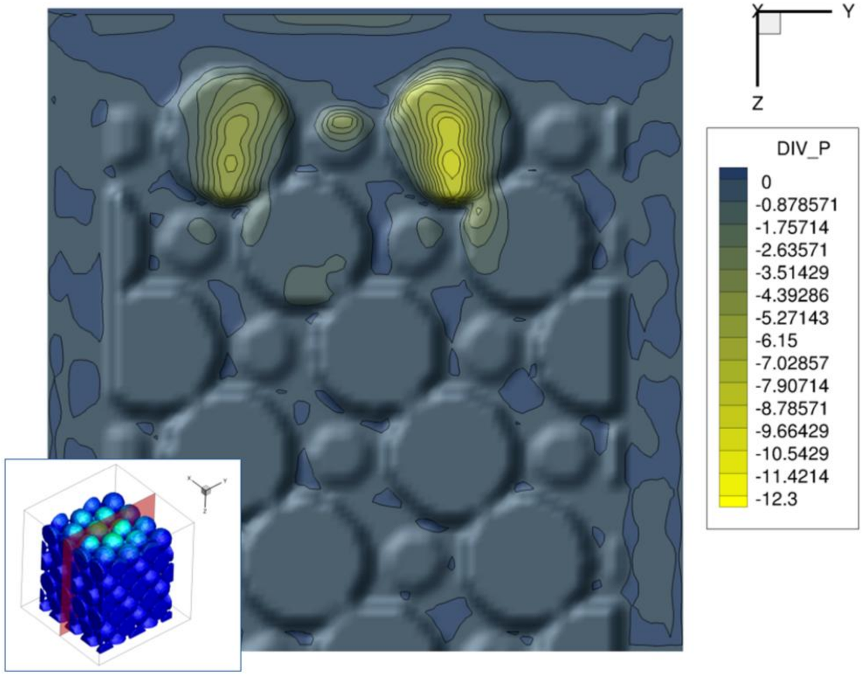
- Selective laser melting and selective laser sintering are processes applied in rapid prototyping and 3D printing technologies. A laser beam is employed to heat powder compacts up to an elevated temperature causing their melting or sintering.
- Small identic particles are packed in a granular bed and heated by a circularly polarized Gaussian laser beam.
- Computations were performed for dielectric materials with zero electric conductivity, ceramics with low conductivity, and metals with high conductivity.



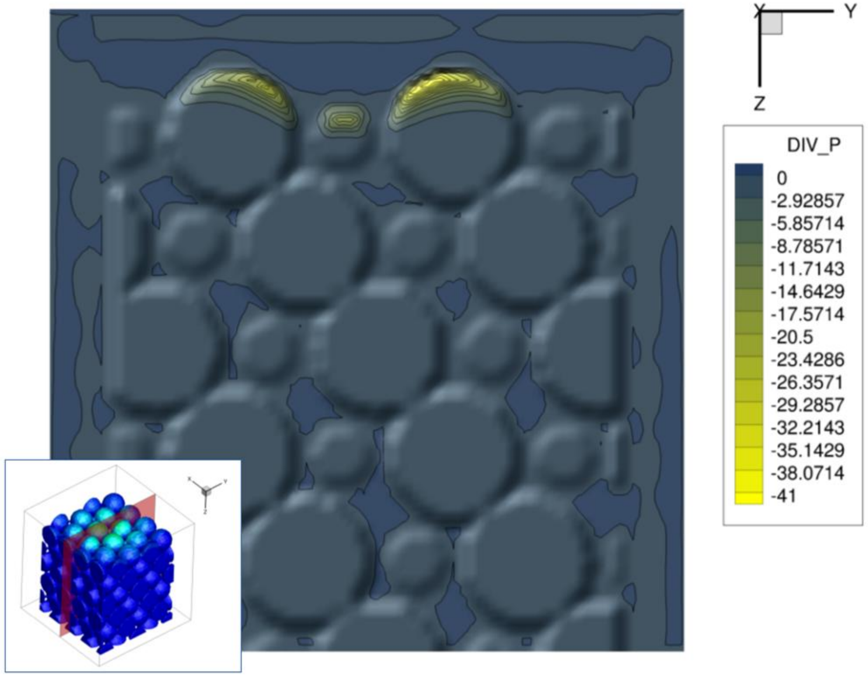
Schematic of laser sintering problem

Laser Melting and Sintering, II

ceramics

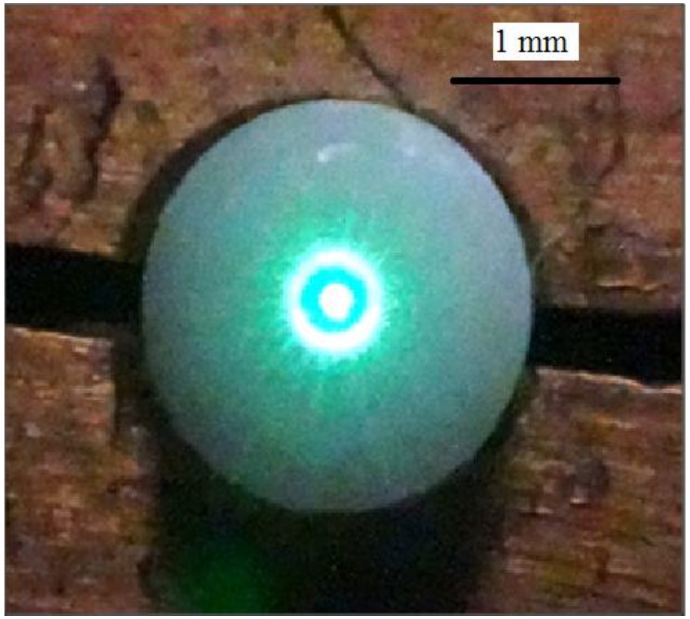


metal



- In ceramic particles laser energy is absorbed within their entire volume.
- In metallic particles, energy is absorbed only by a particle part turned toward the incident radiation.

Fiber-coupled liquid crystal system, I

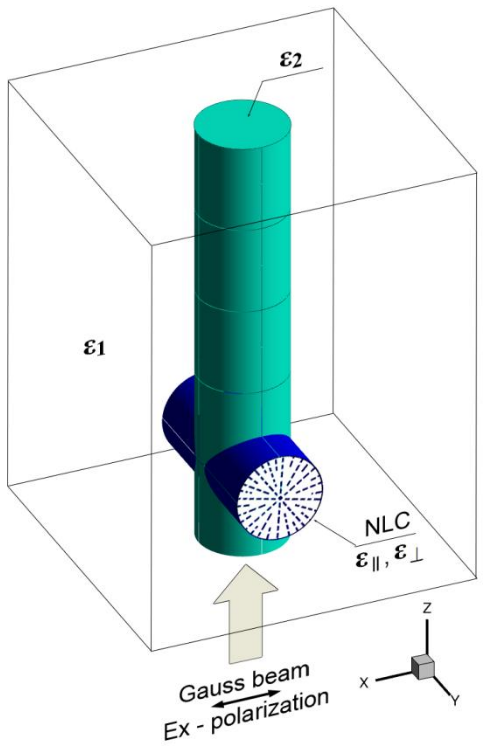


Third harmonic generation in LC droplet at the end face of an optical fiber. The source is a femtosecond laser beam with λ=1560 nm. The conversion efficiency ≈ 15%

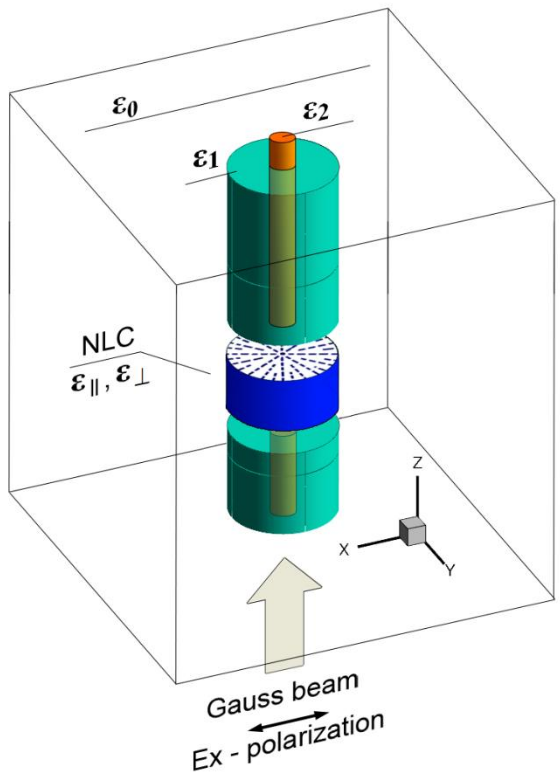
- Due to anomalously high values of nonlinear susceptibilities of liquid crystals (LCs) they can be used to convert and control laser radiation.
- Recently a research team from ***Institute of Laser Physics*** (Novosibirsk, Russia), ***Novosibirsk State University*** and ***Aston Institute of Photon Technologies*** (UK) proposed to use a microscopic (2–8 μm) LC system placed inside the optical fiber as an optical trigger and a converter of EM radiation.
- This integrated, fiber-coupled LC system was simulated numerically in two configurations. In both the cases it is proposed the director distribution in LC contains a linear singularity, the ***disclination*** of strength +1.

Fiber-coupled liquid crystal system, II

- Two configurations of fiber-coupled LC system were considered: one with cylindrical cavity filled with LC and another with a plane layer of LC.



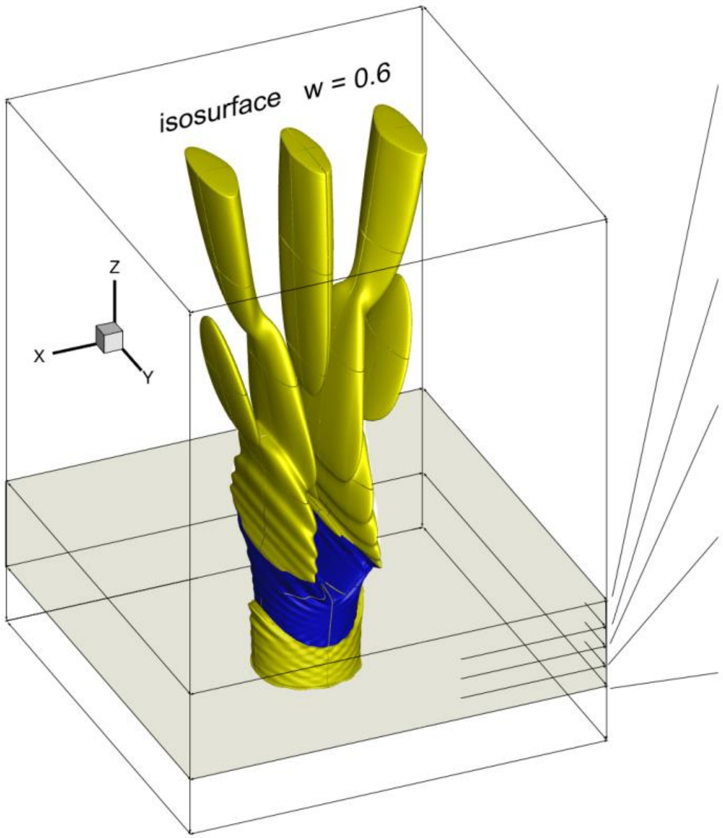
Cylindrical cavity,
$2.7 \cdot 10^8$ cells and
80 cores used



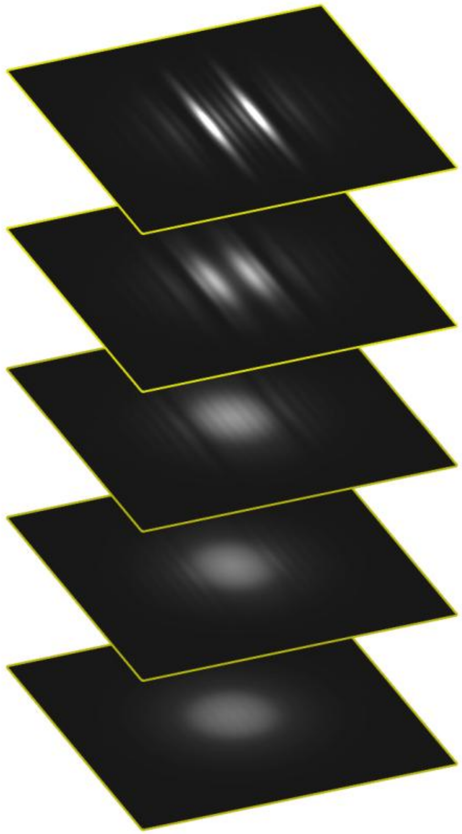
Plane layer,
$4.85 \cdot 10^8$ cells and
144 cores used

Fiber-coupled liquid crystal system, III

EM field energy distribution for the cavity filled with LC.



Isosurface, 0.6 w_{max}

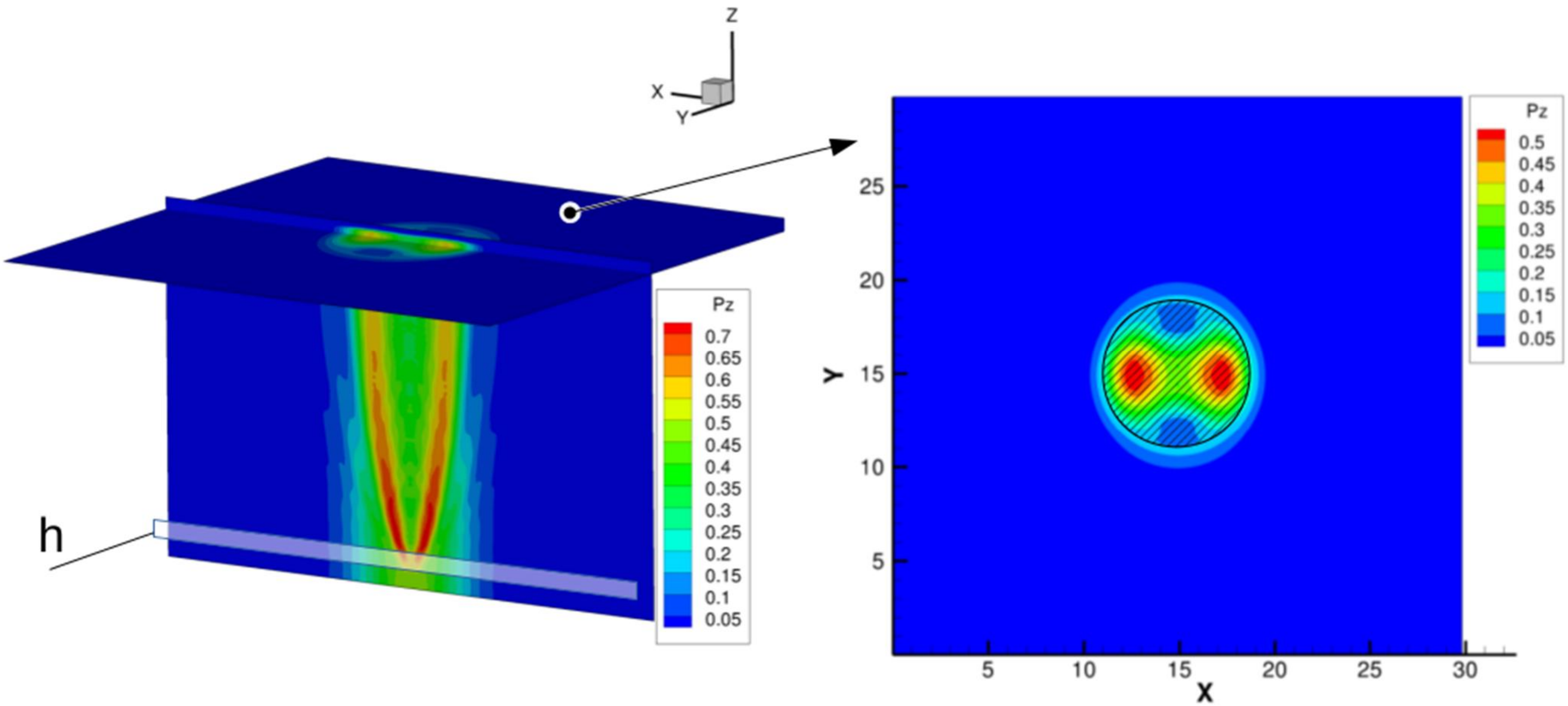


Surface distributions
in 5 cross-sections

The configuration has serious drawbacks: the radiation is focused behind the cavity so that the optical fiber can burn out at high powers of the laser pulse, in addition a significant portion of the radiation is scattered outside the fiber core

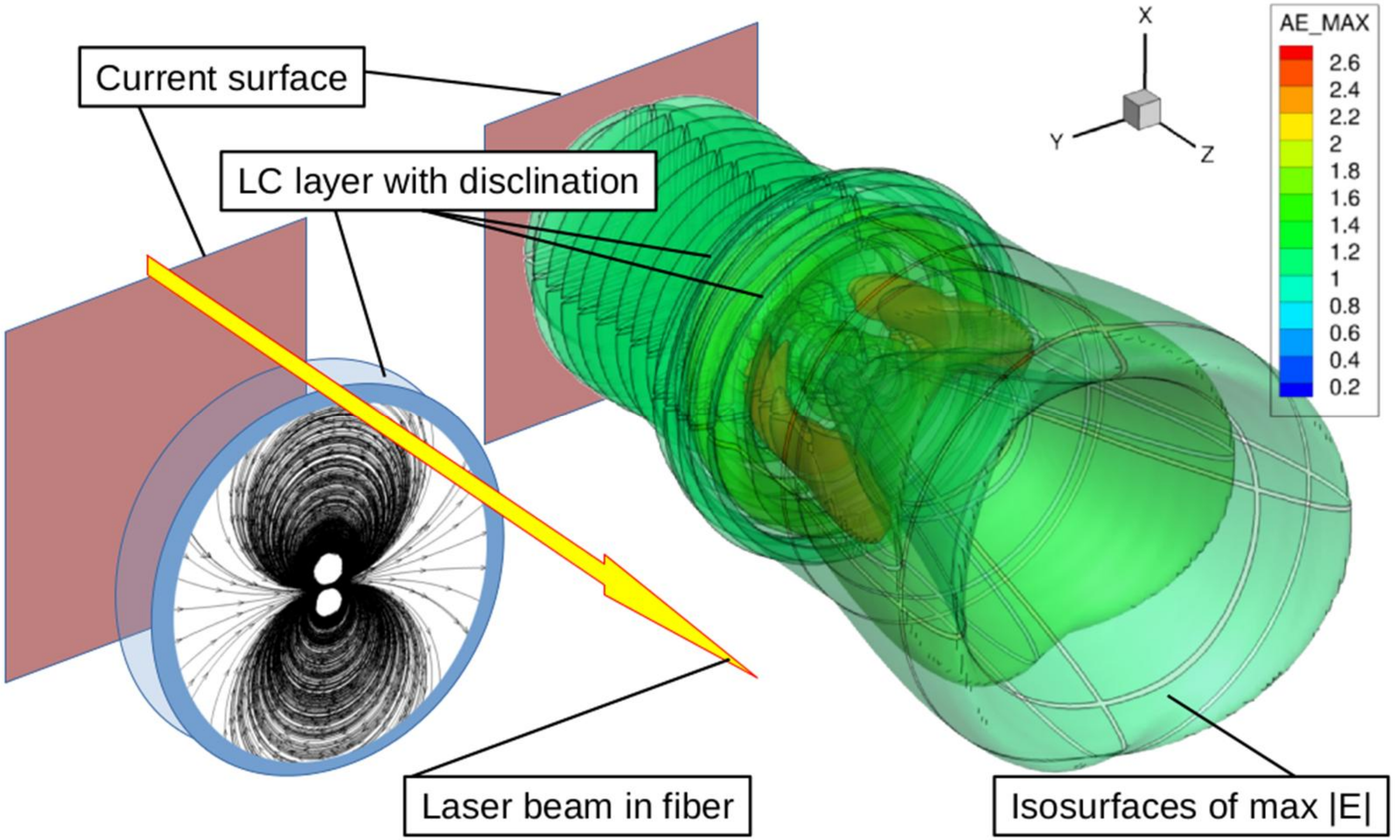
Fiber-coupled liquid crystal system, IV

Distributions of longitudinal component of energy flux density in different cross-sections for the plane layer of LC.



- No significant scattering of radiation was observed for this configuration, which makes it preferrable.

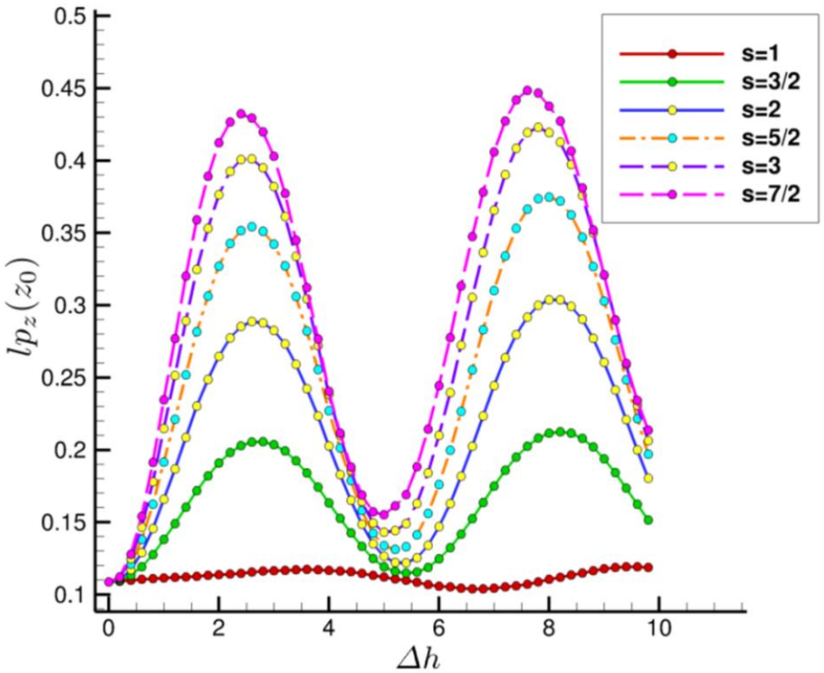
Generation of twisted optical beams, I



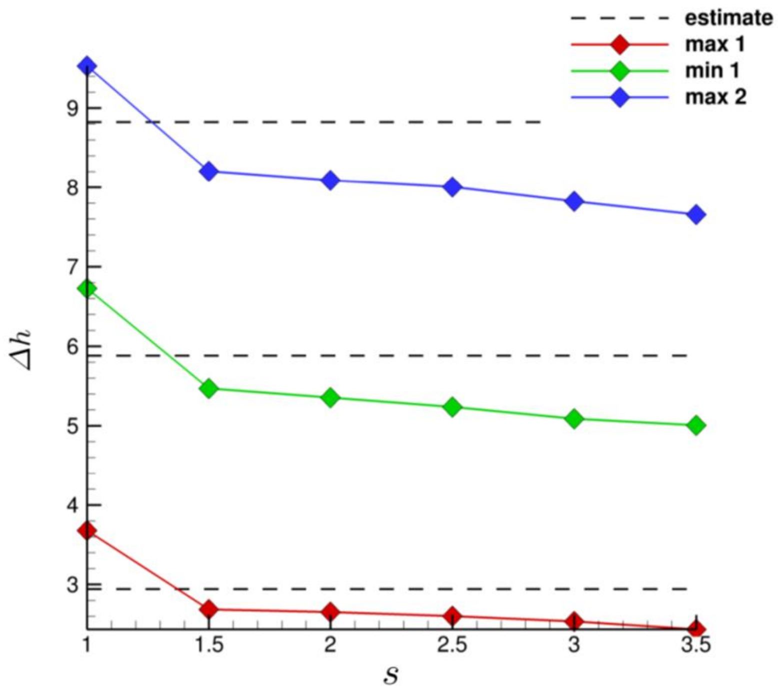
- Optical vortices can be effectively generated at the interaction of light with LCs. The advantage of this approach is the possibility to change the parameters of the output beam dynamically.

Generation of twisted optical beams, II

The transferred angular momentum (AM) depends non-monotonically on the gap width, the beam is twisted and untwisted nearly periodically.



Dependence of the transferred AM momentum portion on the gap width at different disclination strengths.



Gap widths producing peak values of transferred AM vs disclination strength

Conclusion

- Nowadays the development of miniature, micron-sized devices and systems is a general trend and optical devices are not an exception. Numerical simulations of such systems are of great importance for their construction and optimization. The simulations are to be performed by solving Maxwell's equations and for many systems under development can already be carried out with modern supercomputers.

Future work

- To develop a new numerical FDTD code for solving Maxwell's equations on hybrid (CPU/GPU) supercomputers using three-level parallezation with CUDA, OpenMP and MPI and implementing the experience from the development of the DSMC (Direct Simulation Monte Carlo) code **SMILE-cu** and the Navier-Stokes code **HyCFS** in Laboratory of Computational Aerodynamics, Khristianovich Institute of Theoretical and Applied Mechamics, Novosibirsk.

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Thank you for your attention!