How HPC helps exploring electromagnetic near fields

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Theoretical Electrical Engineering

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CeOPP

Deutsche Forschungsgemeinschaft DFG

Sonderforschungsbereich TRR 142

Outline

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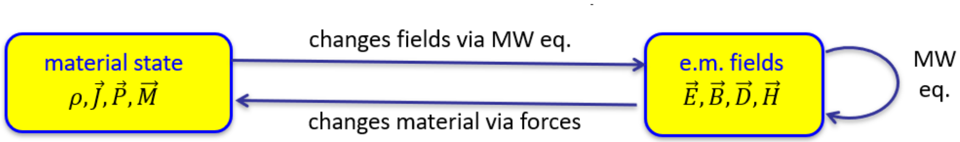
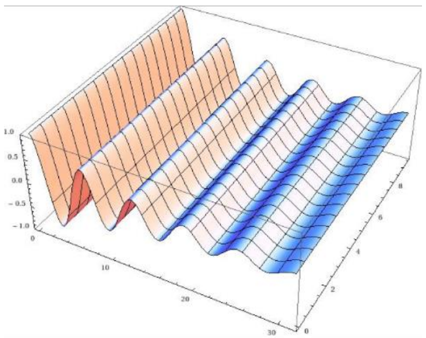
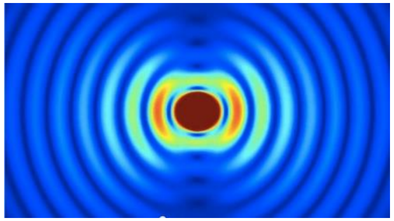
- Maxwell equations



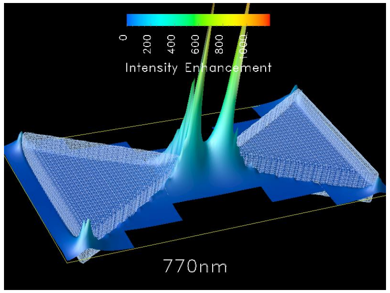
- some analytical solutions



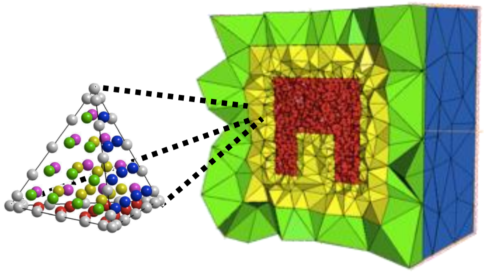
  - homogeneous media
  - point-like sources



- challenges for wavelength-sized structures



- examples from the TET group



Maxwell equations

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Starting point of this talk are the **macroscopic Maxwell equations:**

$$\operatorname{div} \vec{D}(\vec{r},t) = \rho(\vec{r},t)$$

Gauss's law
(Electric charges are the source of electro-static fields)

$$\operatorname{div} \vec{B}(\vec{r},t) = 0$$

Gauss's law for magnetism
(There are no free magnetic charges/monopoles)

$$\operatorname{curl} \vec{E}(\vec{r},t) = -\partial_t \vec{B}(\vec{r},t)$$

Faraday's law of induction
(changes in the magnetic flux ⇔ electric ring fields)

$$\operatorname{curl} \vec{H}(\vec{r},t) = \partial_t \vec{D}(\vec{r},t) + \vec{J}(\vec{r},t)$$

Ampere's law with Maxwell's addition
(currents and changes in the electric flux density ⇔ magnetic ring fields)

$\vec{E}$	electric field strength	$\vec{H}$	magnetic field strength
$\vec{D}$	electric flux density	$\vec{B}$	magnetic flux density
$\vec{P}$	macroscopic polarization	$\vec{P}$	magnetic dipole density
ρ	free electric charge density	$\vec{J}$	free electric current density

$$\partial_t := \frac{d}{dt}$$

$\varepsilon_0 = 8.85 \cdot 10^{-12} \frac{C^2}{Nm^2}$ vacuum permittivity

$\mu_0 = 4\pi 10^{-7} \frac{N}{A^2}$ vacuum permeability

Maxwell theory

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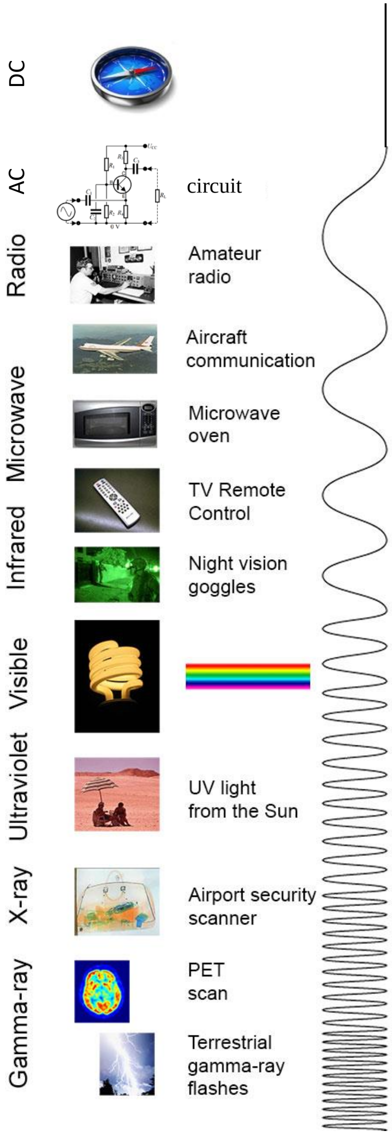

- magnetism (earth, compass)
- binding force between electrons & nucleus => atoms
- binding between atoms => molecules and solids
- <1 kHz: electricity, LF electronics
- antennas, radiation: radio, satellites, cell phones, radar
- metallic waveguides: TV, land-line communication, power transmission, HF electronics
- lasers, LEDs, optical fibers
- medical applications
- X-Ray scanning
- astronomy

Full range of effects are described by the same theory: Maxwell equations

However the material response depends strongly on the frequency.

http://imagine.gsfc.nasa.gov/Images/science/EM_spectrum_full.jpg, http://imagine.gsfc.nasa.gov/Images/science/EM_spectrum_full.jpg

Maxwell equations

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Ampere's law with Maxwell's addition
(currents and changes in the electric flux density ⇔ magnetic ring fields)

Together with the **constitutive/material relations**:

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P}$$

$$\vec{H} = \frac{1}{\mu_0}\vec{B} - \vec{M}$$

$\vec{E}$	electric field strength	$\vec{H}$	magnetic field strength
$\vec{D}$	electric flux density	$\vec{B}$	magnetic flux density
$\vec{P}$	macroscopic polarization	$\vec{P}$	magnetic dipole density
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Material models

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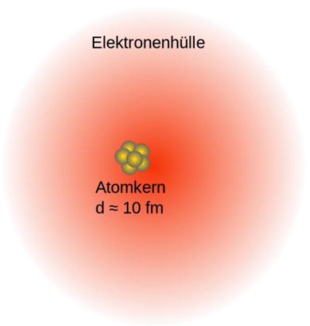
The e.m. fields originate from free charges $(\rho, \vec{J})$ and bound charges $(\vec{P}, \vec{M})$.

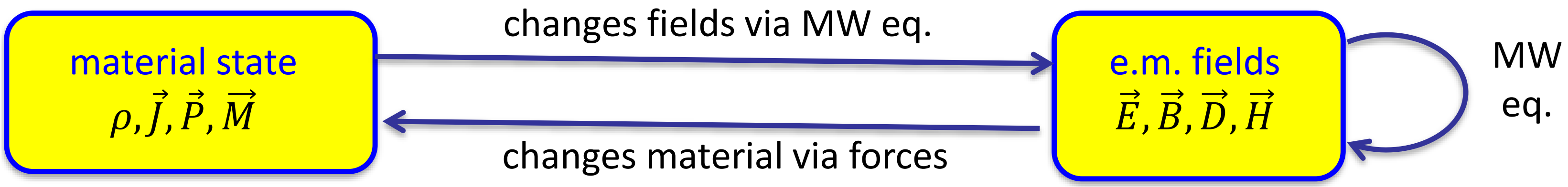


https://de.wikipedia.org/wiki/Datei:Polarisiertes_Atom.svg

The charges, however, feel a force via the electromagnetic fields:

$$\vec{F} = \underbrace{q\vec{E}}_{\text{Coulomb force}} + \underbrace{q\vec{v} \times \vec{B}}_{\text{Lorentz force}}$$

This force accelerates the charges leading to changes in $\rho, \vec{J}, \vec{P}$, and $\vec{M}$:



⇒ The material quantities are functionals of the fields, i.e. they may depend on the fields at all other points in space in time.

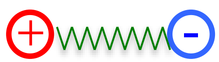
⇒ complex spatio-temporal coupled dynamics!

Material models

With a few assumptions (linearity, locality, causality, achirality, time invariance), the material relation for $\vec{D}$ can be written in frequency space as simple proportionality:

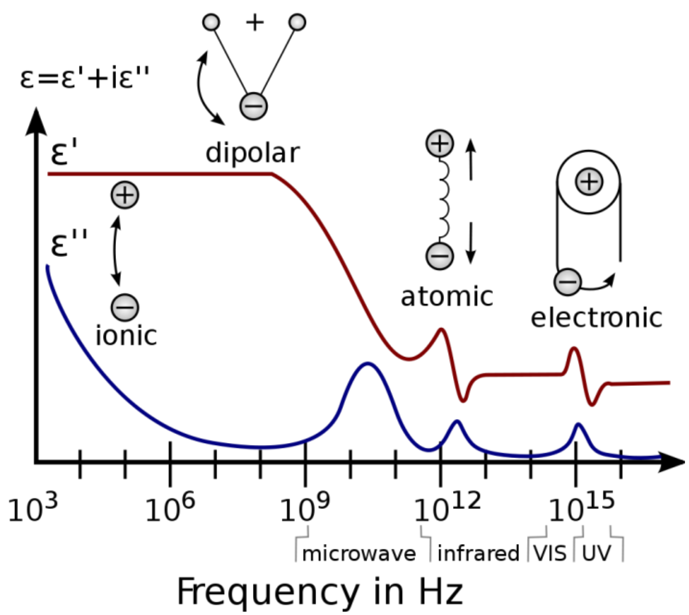
$$\vec{D}(\vec{r},\omega) = \vec{\vec{\varepsilon}}(\vec{r},\omega)\vec{E}(\vec{r},\omega)$$

In non-conducting dielectric materials the restoring force on bound charges often scales mostly linear with the external force (Hooke's law, linear spring). This leads to a (damped) harmonic oscillator called **Lorentz model.**



$$\ddot{\vec{u}} + \gamma\dot{\vec{u}} + \omega_0^2\vec{u} = \alpha\vec{E} \quad \Rightarrow \varepsilon(\omega) = \varepsilon_0 + \frac{s}{\omega^2 - \omega_0^2 - j\omega\gamma}$$

In solids there are many types of oscillations (electronic, atomic, dipolar, ionic) of different frequencies which superpose, i.e. sum up:



real part ε' → dispersion

imaginary part ε'' → damping

https://en.wikipedia.org/wiki/Permittivity

The wave equation

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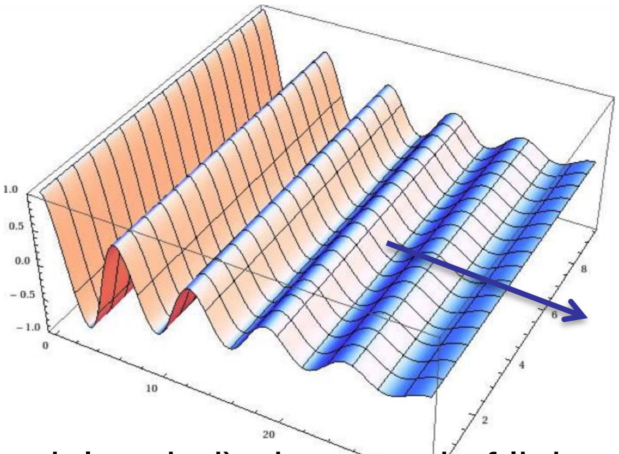
Assuming a spatial homogeneous material, i.e. spatially constant $\tilde{\varepsilon}$ & μ, and no free charges one can derive the wave equation, in frequency domain called **Helmholtz equation**:

$$\Delta \vec{E}(\vec{r},\omega) + \omega^2 \tilde{\varepsilon}(\omega)\mu(\omega)\vec{E}(\vec{r},\omega) = j\omega\mu(\omega)\vec{J}_e(\vec{r},\omega)$$



One set of solutions are **plane waves** (for $J_e = 0$): $e^{j\omega t - j\vec{k}\cdot\vec{r}}$

The (circular) frequency ω and wave number k are linked via a **dispersion relation:** $k^2 = \omega^2\tilde{\varepsilon}(\omega)\mu(\omega)$.

The real part $\beta = \mathrm{Re}\, k$ determines the wavelength $\lambda = 2\pi/\beta$ (i.e. spatial period), the speed of light in a medium $v_{ph} = \omega/\beta$, and it's derivative the group velocity $v_{gr} = \partial\omega/\partial\beta$

The imaginary part $\alpha = \mathrm{Im}\, k$ determines damping effects.

Superpositions lead to more complex field patterns (interference).

Interfaces

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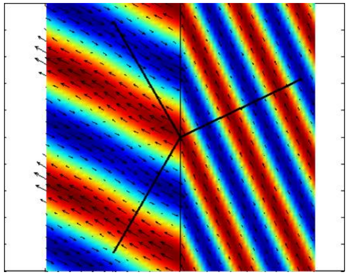
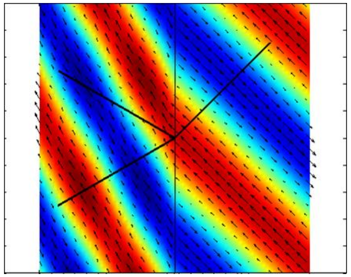
Things get interesting at interfaces between homogeneous media:

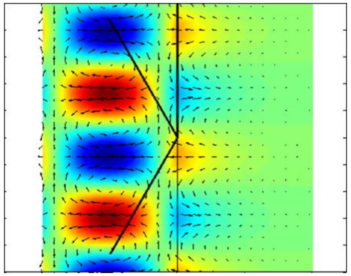
Refraction: $\varepsilon_1 < \varepsilon_2 \Rightarrow$ towards normal $\varepsilon_1 > \varepsilon_2 \Rightarrow$ away from normal





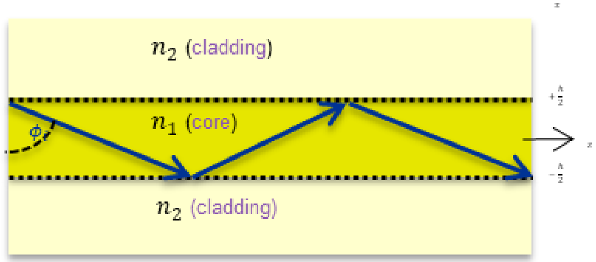
https://en.wikipedia.org/wiki/Total_internal_reflection#/media/File:Total_internal_reflection_of_Chelonia_mydas.jpg

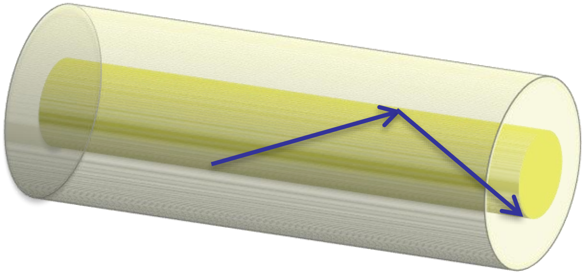
For $\varepsilon_1 > \varepsilon_2$ total reflection can occur above a critical angle: (100% reflection, evanescent decaying field in media 2)

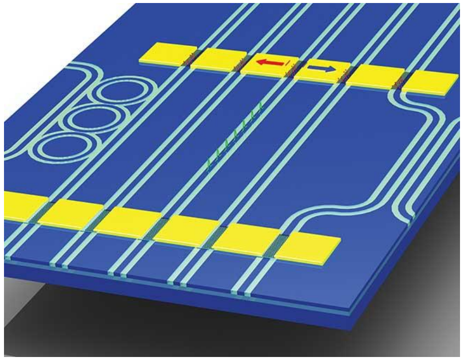


https://www.flickr.com/photos/jtbss/9393445794

This is the basis for wave guiding in dielectrics $\Rightarrow$ fibre optics, integrated photonics







https://www.photonics.com/Articles/Integrated_Photonics_A_Tale_of_Two_Materials/a60862

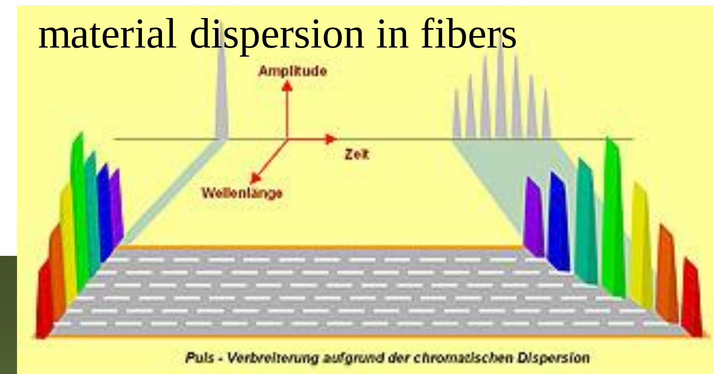
Dispersion

The material parameter $\varepsilon(\omega)$ depends on frequency

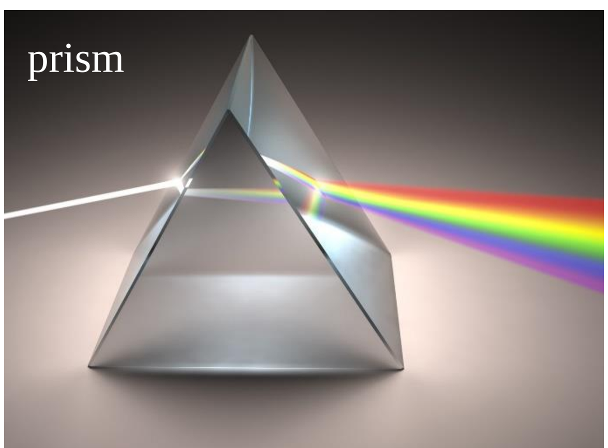
⇒ strength of refraction & speed of light differs for spectral components

examples:

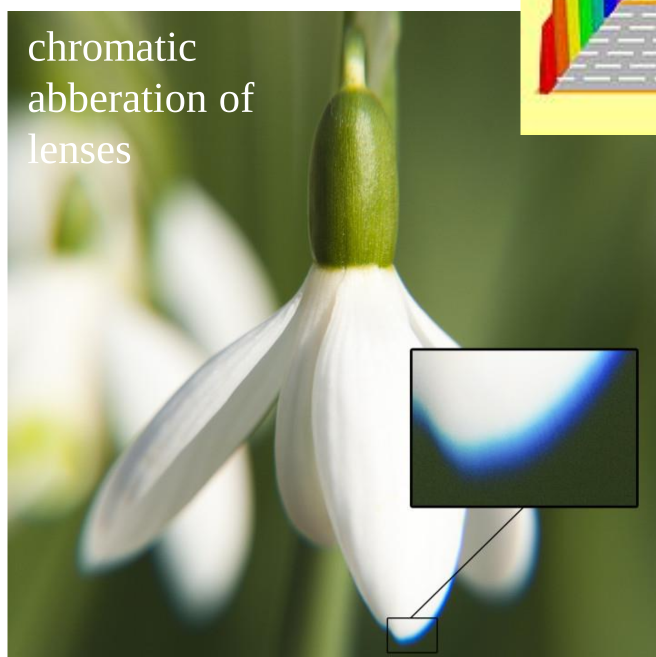
http://avax.news/touching/Simply_Some_Photos_Rainbow_04-12-2014.html



https://www.opternus.de/anwendungsgebiete/optische-messtechnik/cd-chromatische-dispersion



https://rivel.com/the-prism-a-full-spectrum-of-color-on-governance-issues/



http://pixxel-blog.de/was-ist-eigentlich-chromatische-aberration/

Tiny particles

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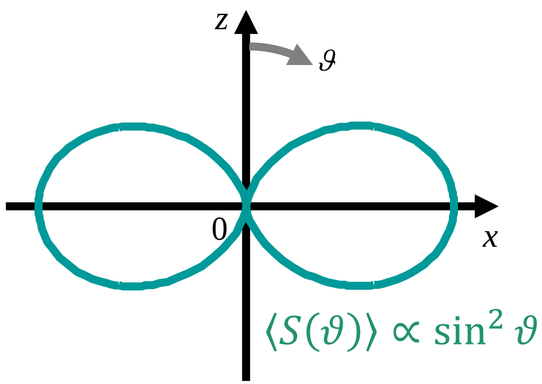
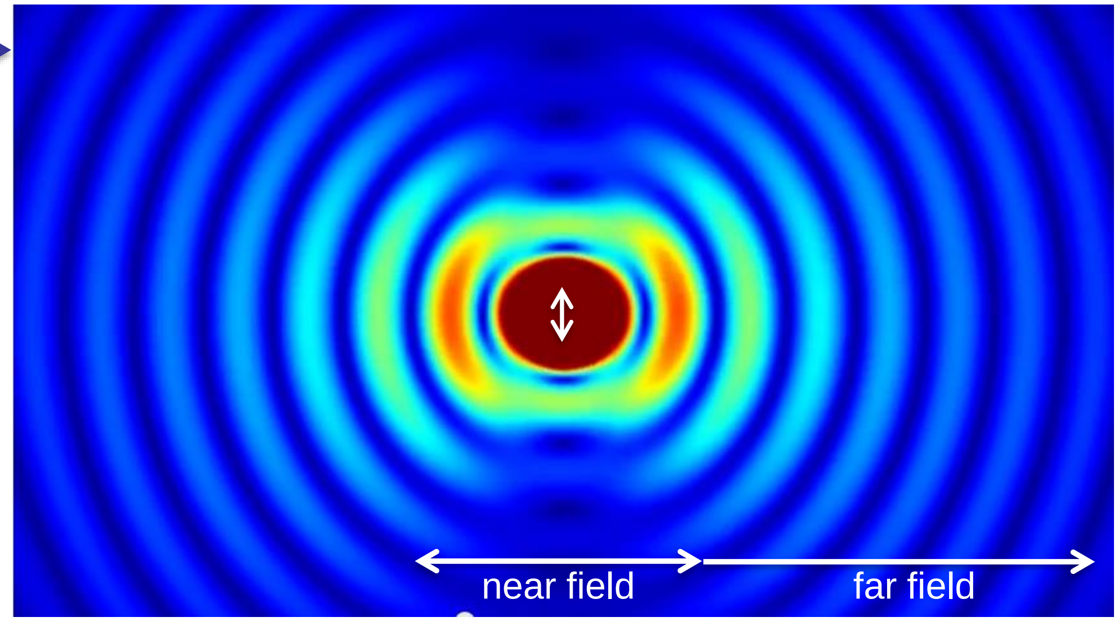
Homogeneous media & simple boundaries ⇒ analytical solutions ⇒ no need for HPC.

How about tiny particles (much smaller than the wavelength), look at point-like emitter:



$|\vec{E}|^2$ →



https://www.youtube.com/watch?v=F3SXmgm2uxM

electric field: $\vec{E}_\vartheta = \frac{p}{4\pi\varepsilon} e^{-jkr}\, k^2 \left(\frac{1}{k^2 r^2} - \frac{2j}{kr}\right) \sin\vartheta$

- $\frac{p}{4\pi\varepsilon} e^{-jkr}$: spherical waves
- k^2: via $k \propto \omega$ frequency dependence
- $\frac{1}{k^2 r^2}$: near field (small for large r)
- $\frac{2j}{kr}$: far field
- $\sin\vartheta$: angular dependence (radiation pattern)

Raleigh scattering

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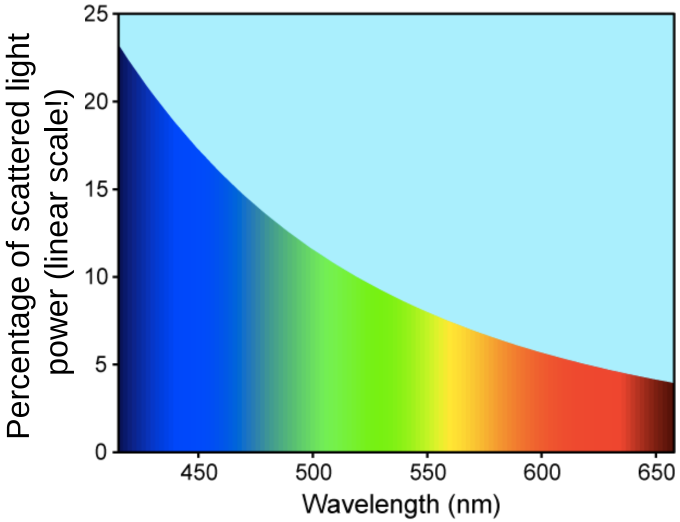
This also explains how e.m. fields scatter off tiny particles (**Rayleigh scattering**):

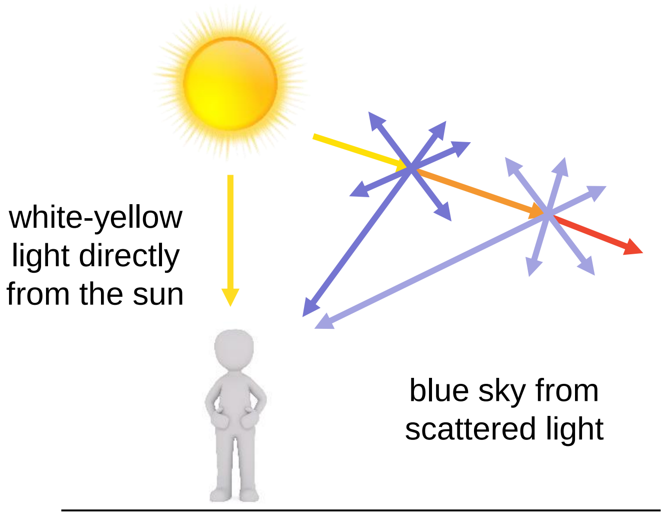
$$P_{scattered}(\omega) \propto \frac{1}{\lambda^4} P_{in}(\omega)$$



https://en.wikipedia.org/wiki/Rayleigh_scattering

Some consequences:

(1) Blue sky



http://www.sciencemadesimple.com/sky_blue.html

Rayleigh Streuung

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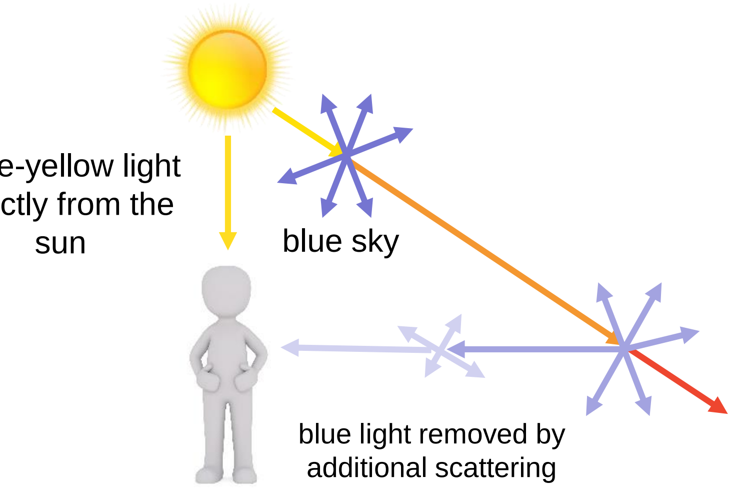
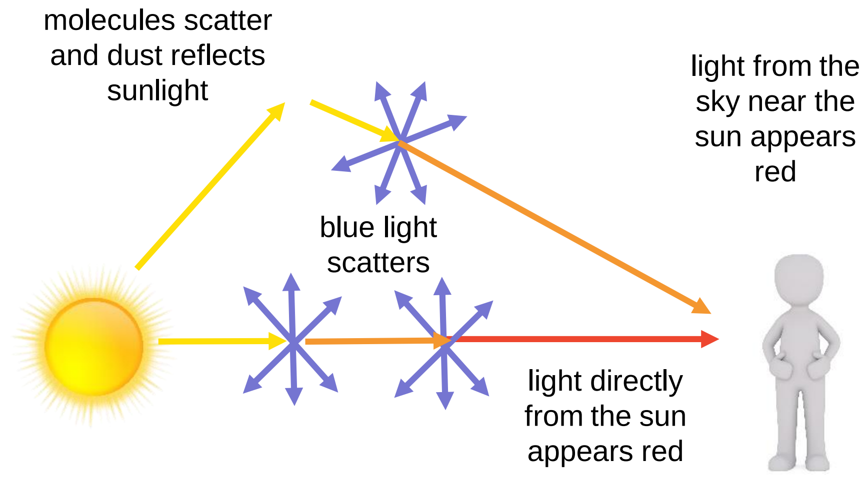
(2) Sky pale/whiter near horizon

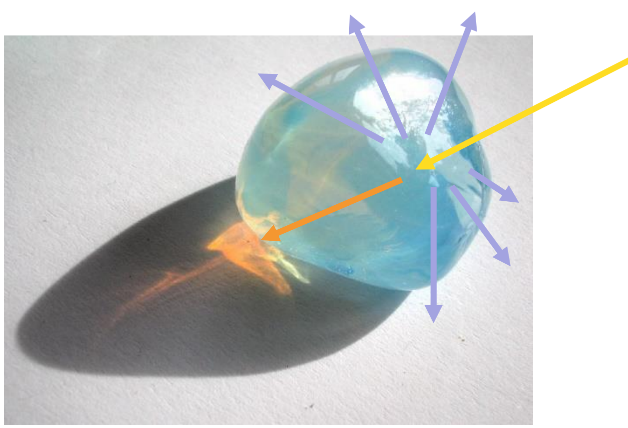


(3) sunsets are red



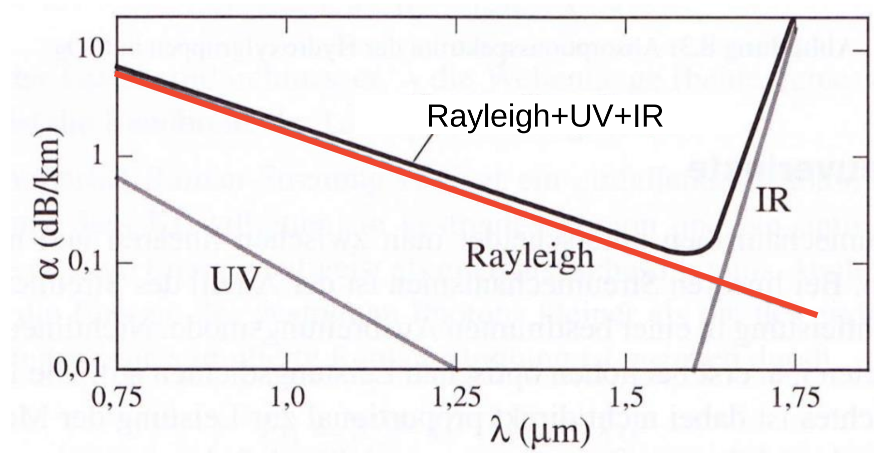
Idee von http://www.sciencemadesimple.com/sky_blue.html

(3) scattering in "milk opal"



https://upload.wikimedia.org/wikipedia/commons/0/0b/Why_is_the_sky_blue.jpg

losses in fibres



Jahns "Photonik"

Tiny particles

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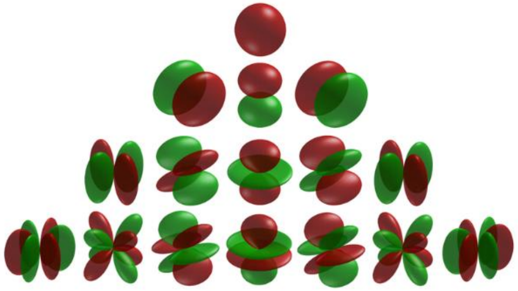
One tiny particle ⇒ no need for HPC.

How about the mesoscopic e.m. "Mie" regime, i.e. particle size ≈ wavelength?

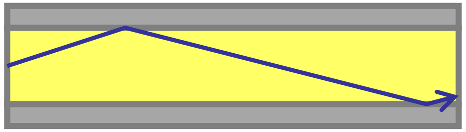
Only few analytical solutions for high symmetry:

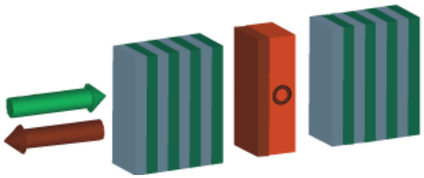
Spherical: Mie solutions,
spherical harmonic functions



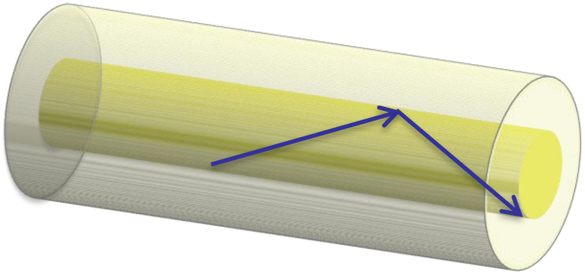
https://de.wikipedia.org/wiki/Kugelfl%C3%A4chenfunktionen

Planar symmetries





Cylindrical



Everything more complex ⇒ numerical simulation

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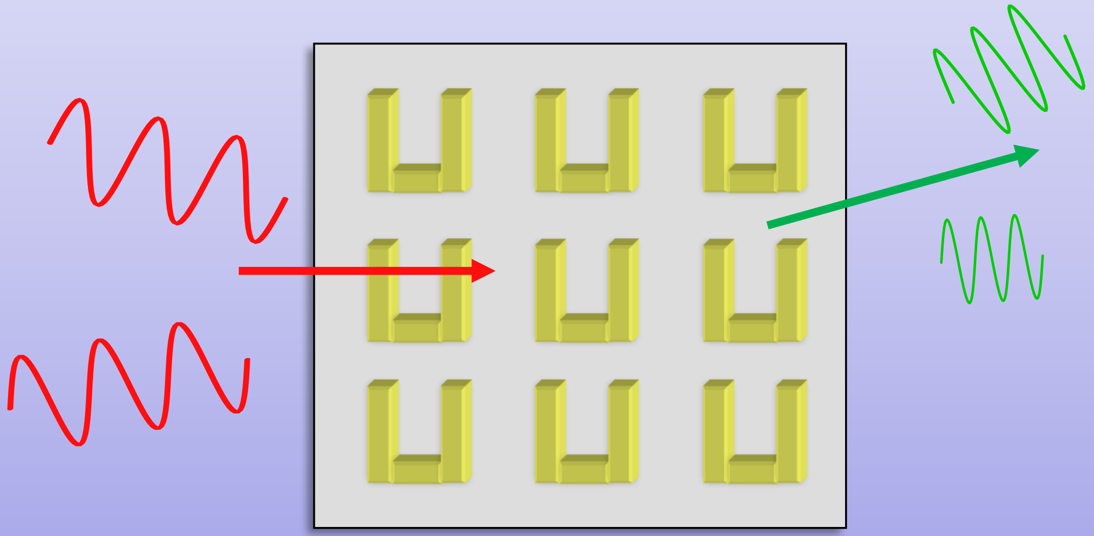
Simulation of the Second Harmonic Generation (SHG) in arrays of gold split ring resonators.

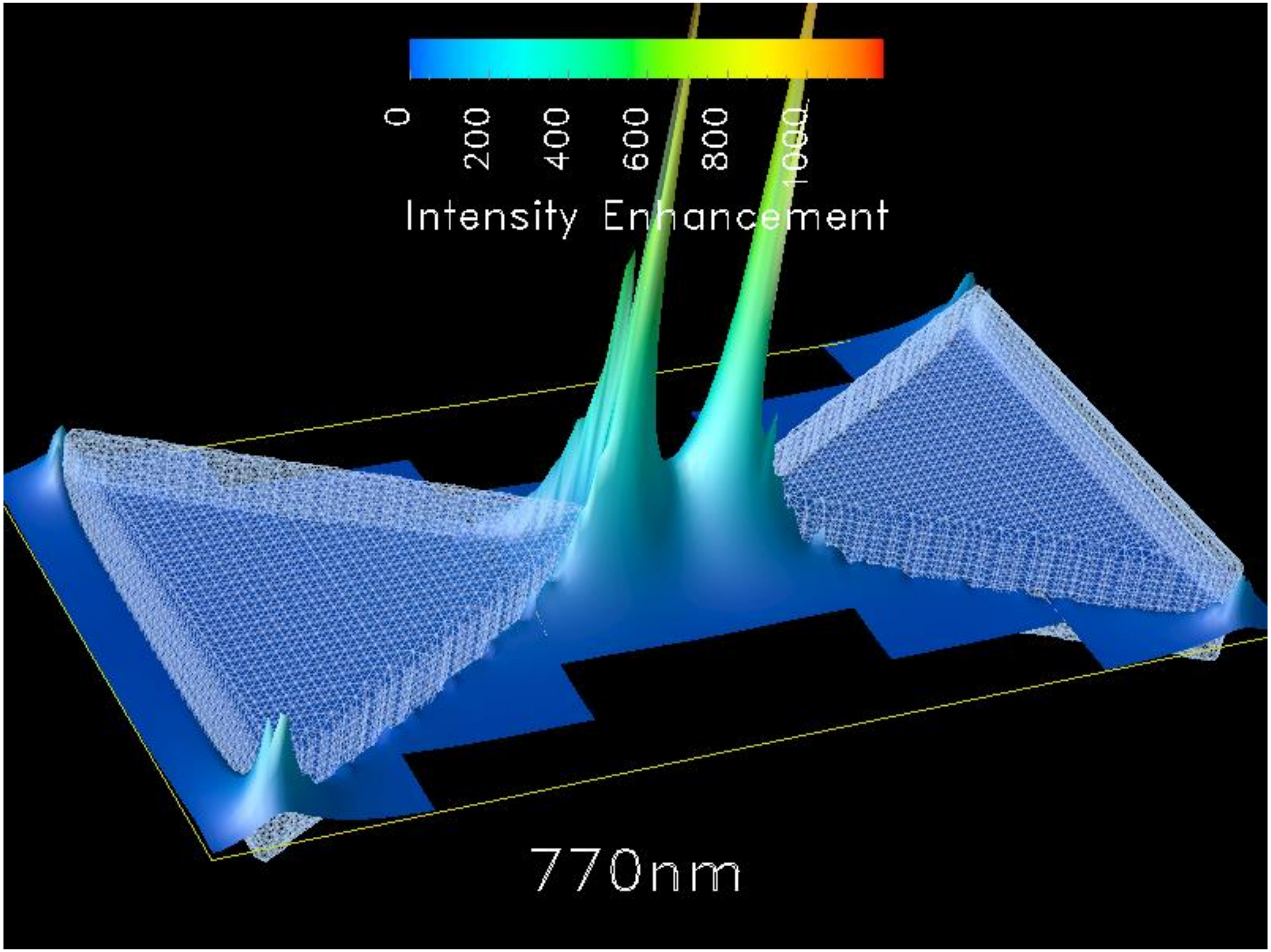
Question for the theory:

Where and how is SHG signal generated?

- Surface?
- Bulk?
- Substrate?
- Depositions?



Challenge: strong variation of fields



© Matthias Reichelt (UPB, NW-P)

Electromagnetic fields are strongly enhanced and vary on extremely short scales

Simulation of nanostructures

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-> **challenges for theory**:

- Strong near field enhancement and extreme field variation,
- Complex optical response of materials (dielectrics and metals): nonlinearites, nonlocality, anisotropy, decoherence,
- Nontrivial short- and long distance coupling.

Requires:

- Advanced nonlinear/nonlocal/anisotropic material models,
- Adaptive mesh time domain PDE solver,
- Efficient parallel implementations.

⇒ All tested available tools failed

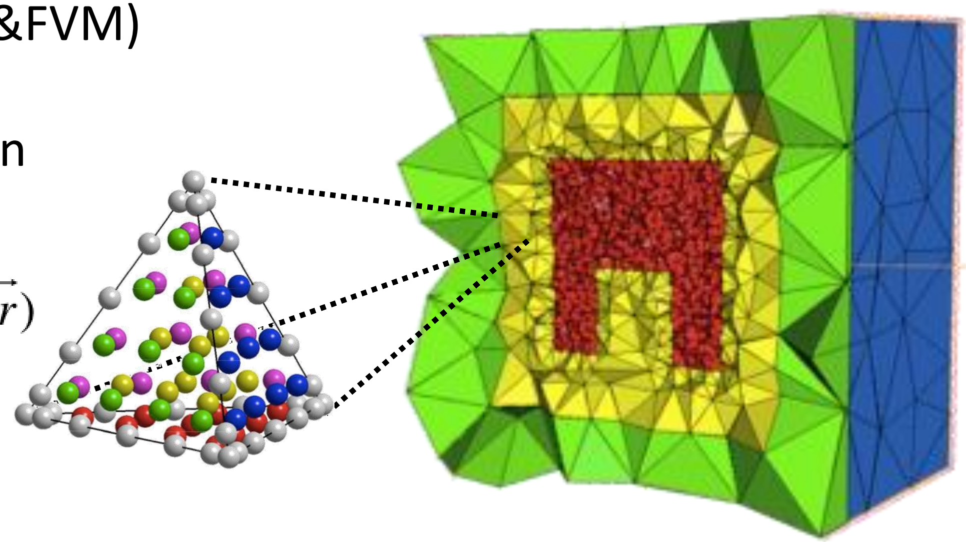
Our numerical method of choice

Nodal Discontinuous Galerkin Time-Domain Method (DGTD)

(unstructured grid, related to FEM&FVM)

Spatial distribution of interpolation nodes in an element

$$q^k(\vec{r},t) \approx \sum_{i=1}^{N} q^k(\vec{r}_i,t) L_i(\vec{r}) = \sum_{i=1}^{N} \widetilde{q_i^k}(t)\varphi_i(\vec{r})$$

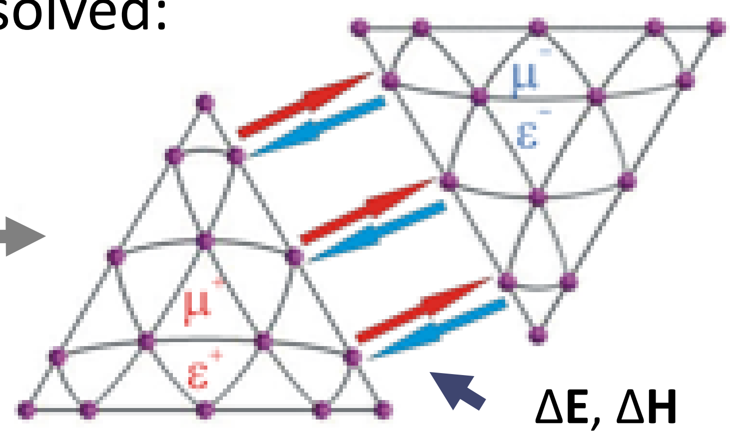


The field components for $\vec{E}$ and $\vec{H}$ are expanded *locally* in each cell.

There Maxwell and material equations are solved:

$$\frac{\partial \mathbf{E}^k}{\partial t} = \frac{1}{\epsilon^k}\left[\mathbf{D}^k \times \mathbf{H}^k + (\mathcal{M}^k)^{-1}\mathcal{F}^k\left[\alpha(\Delta\mathbf{E} - \hat{n}(\hat{n}\cdot\Delta\mathbf{E})) + Z^{+}\hat{n} \times \Delta\mathbf{H}\right]/\bar{Z}\right]$$

Then exchange of e.m flux.



Hesthaven, Warburton, Springer Book (2007)
Busch et al, Laser & Photonics Reviews (2011)

Properties of the DGTD method

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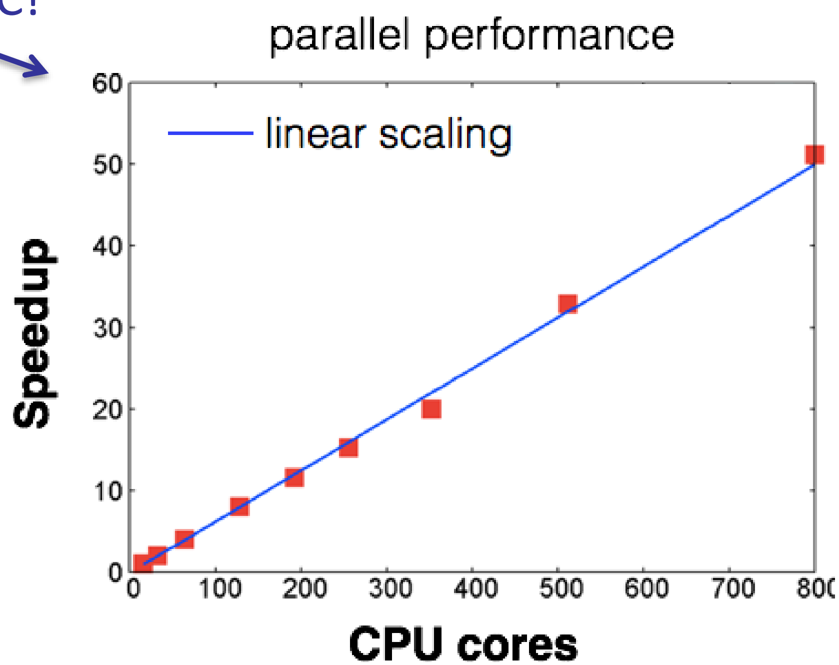
The Discontinuous Galerkin Time Domain (DGTD) method:

- ☺ Unstructured, adaptive mesh -> multiscale, multiphysics,
- ☺ full geometrical flexibility (substrate, materials, etc)
- ☺ direct incorporation of nonlinear material equations in TD,
- ☺ stability can be proven, even for some nonlinearities,
- ☺ excellent parallel scaling,
- ☹ complex method, effort of implementation,
- ☹ high cost of mesh generation.

HPC!



Cooperations with C.Plessl/PC2,
BMBF project HighPerMeshes

Research topics in my group

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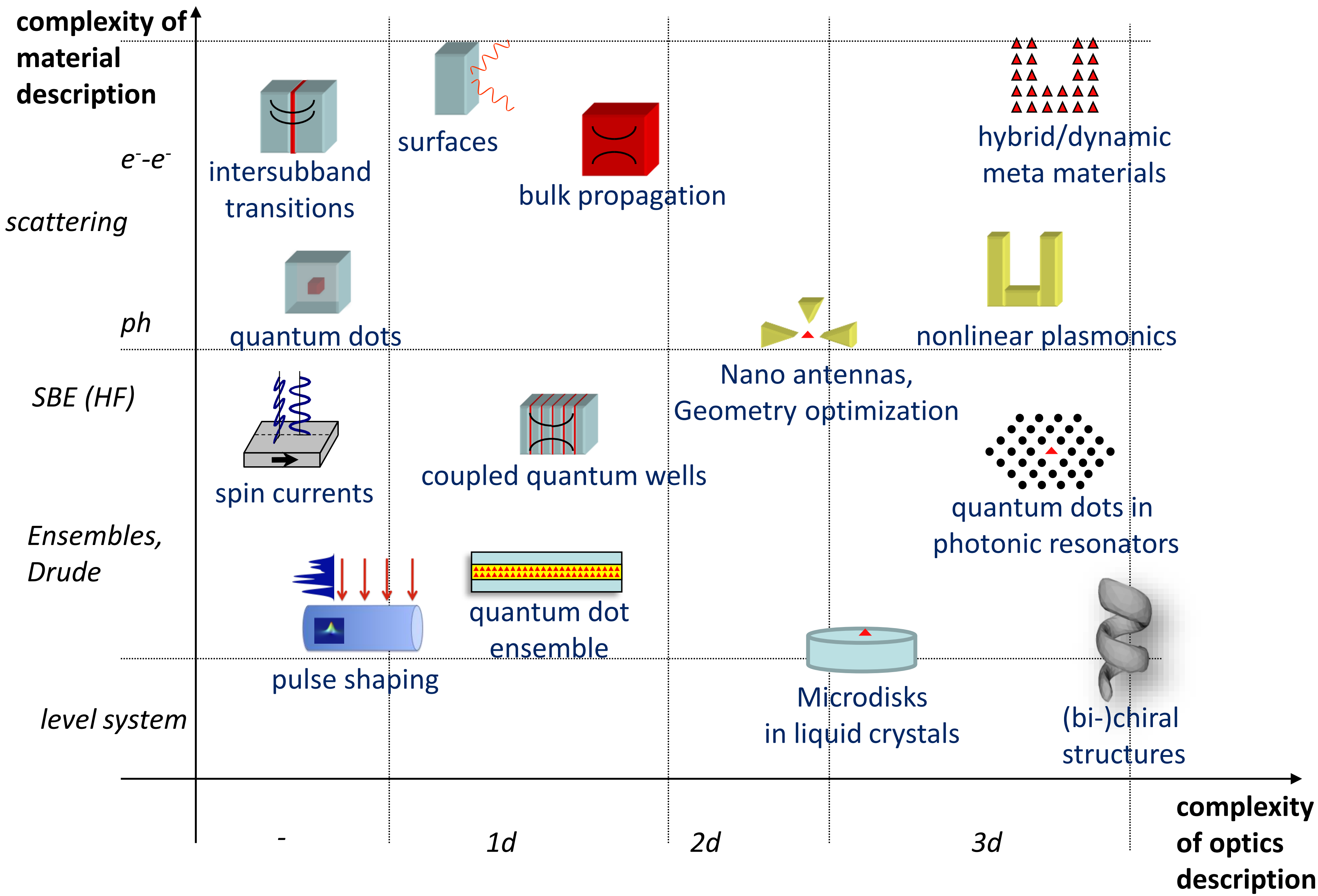

Higher Harmonic Generation

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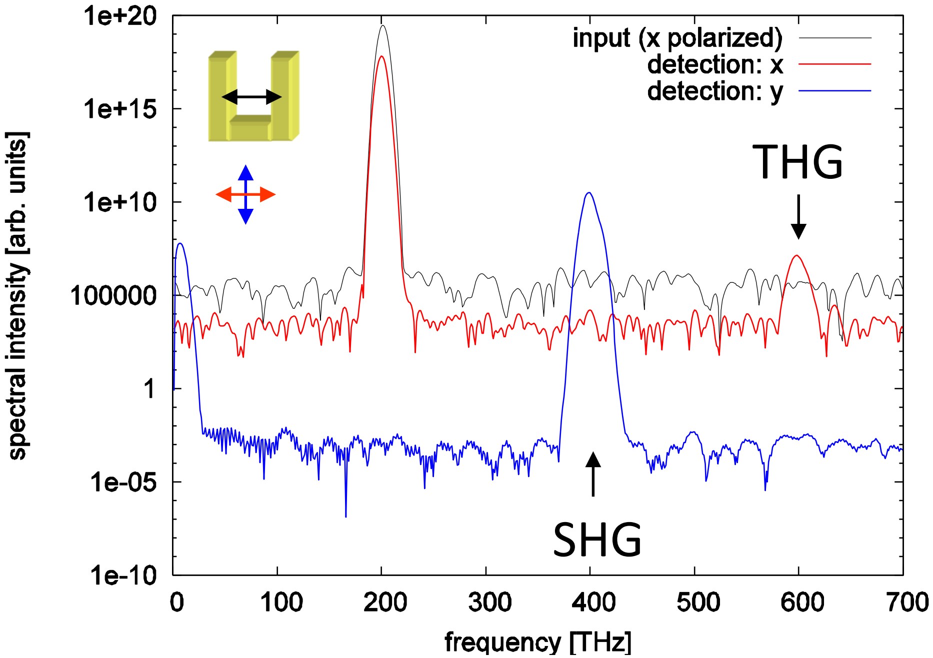
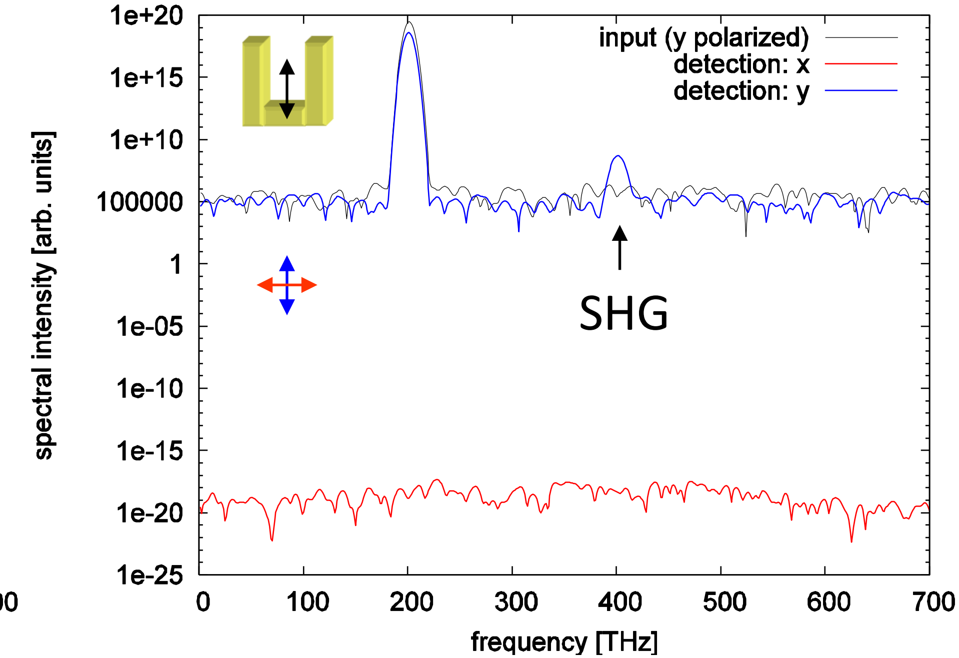
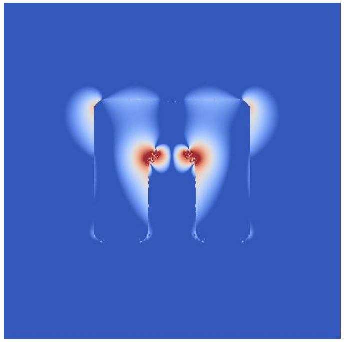
Simulated emission using symmetrized grids:





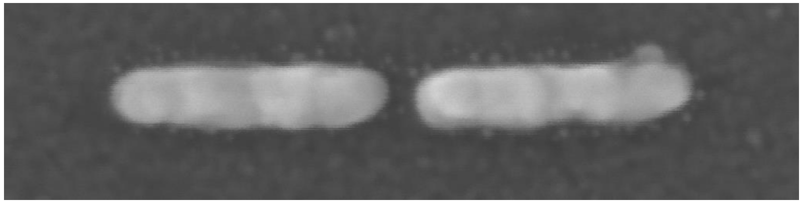
- **SHG** only in symmetry-broken direction (y)
  - (Semi-classical) Fermi pressure negligible
  - SHG mainly generated at edges
  - Advection and charge shift counteracting, still larger than $\vec{J} \times \vec{B}$ nonlinearity.
- Third harmonic generation (**THG**) in excitation direction



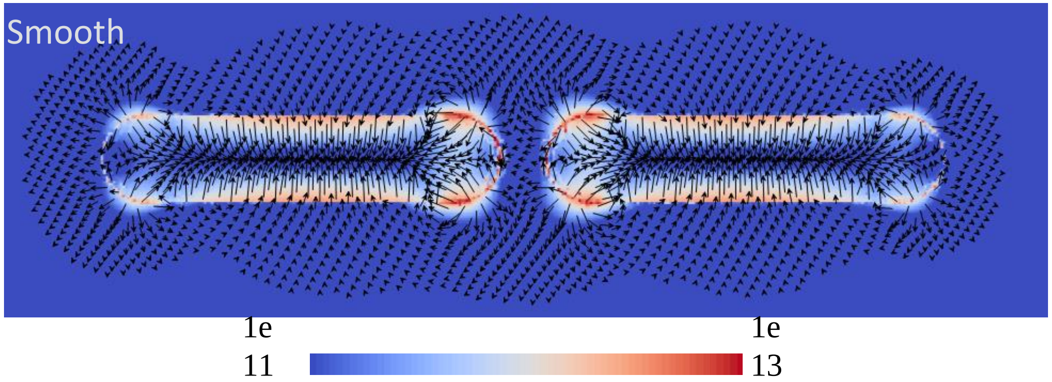
near field

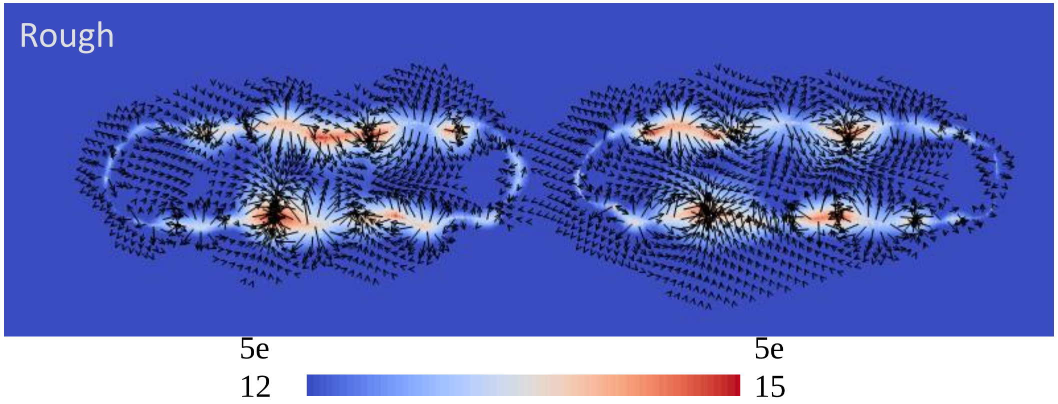
related structure, single particle ("nanoantenna")

experiment:



Model roughness, near fields at rough surface:





This explained the experimentally observed strong SHG signal.

[Light: Science & Applications 2016]

Application of TD-DG to dust particles

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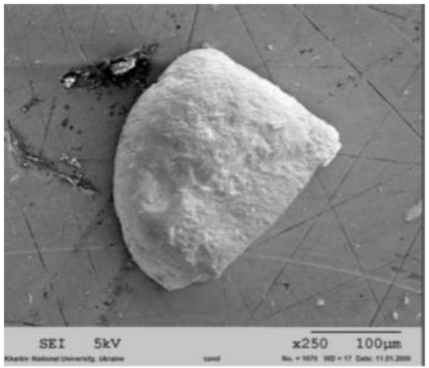
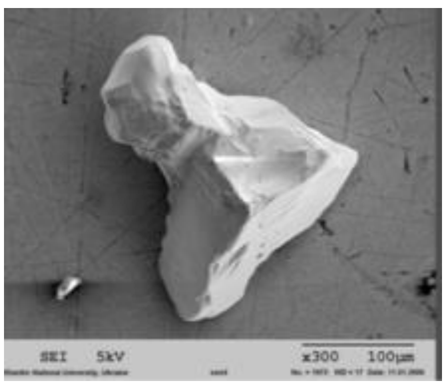
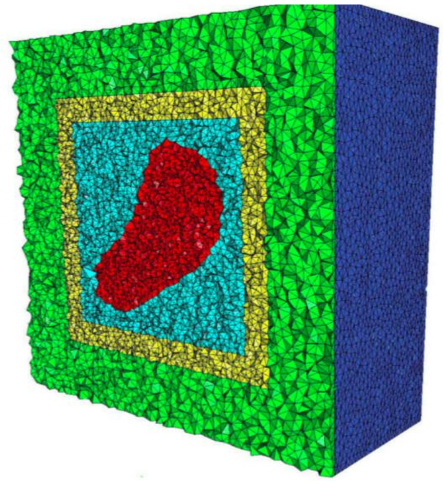
Die Universität der Informationsgesellschaft

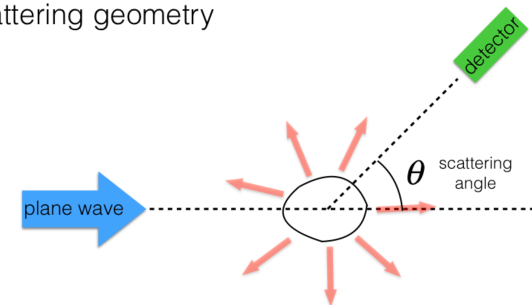
Scattering of microwaves at larger particles ($r \ll \lambda$), e.g. at interplanetary dust and atmospheric ice particles:

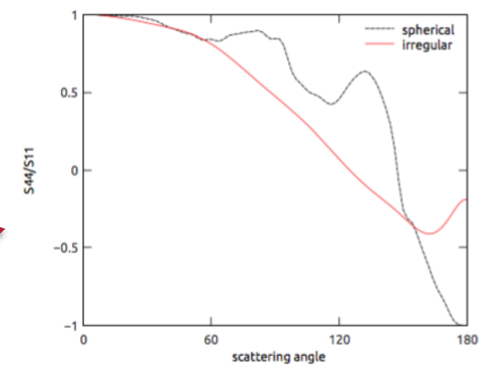






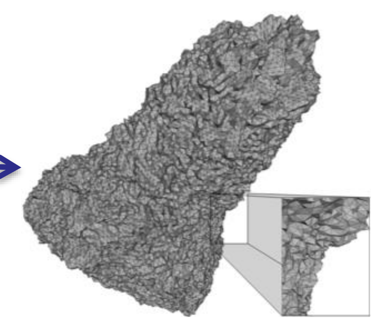
Scattering geometry





e.g. used to determine size distribution of cometary dust from radar measurements

Large particles and rough surfaces are numerically very demanding → "Discontinuous Galerkin method" (lecture)



Application of TD-DG to dust particles

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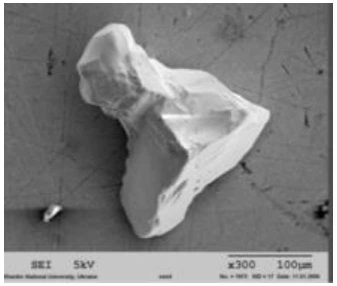
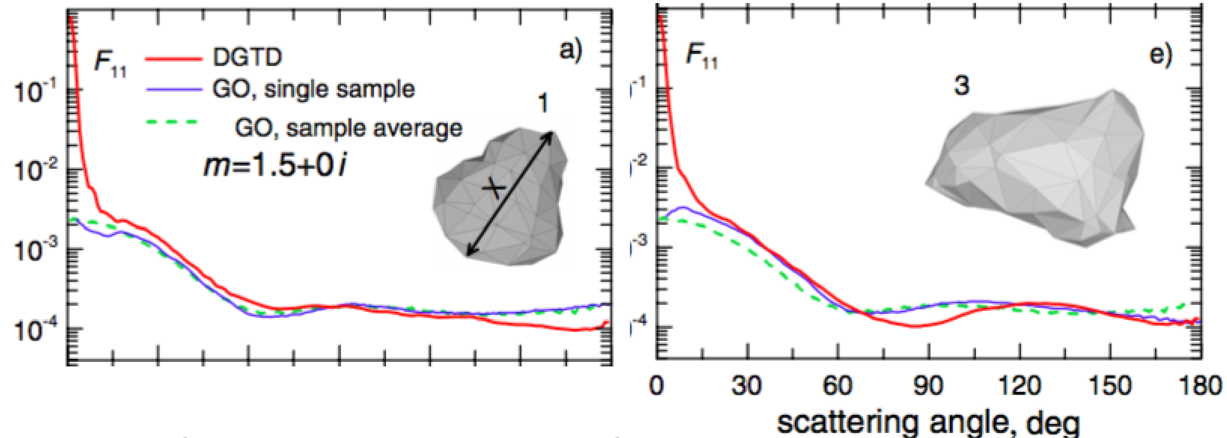
X=60:

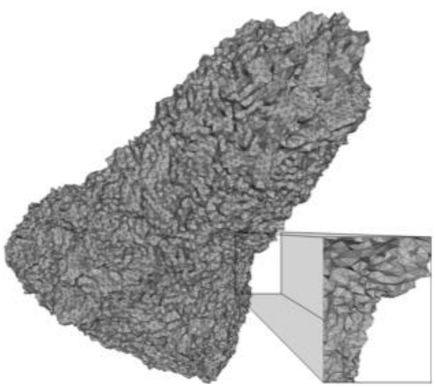


TD-DG & GO

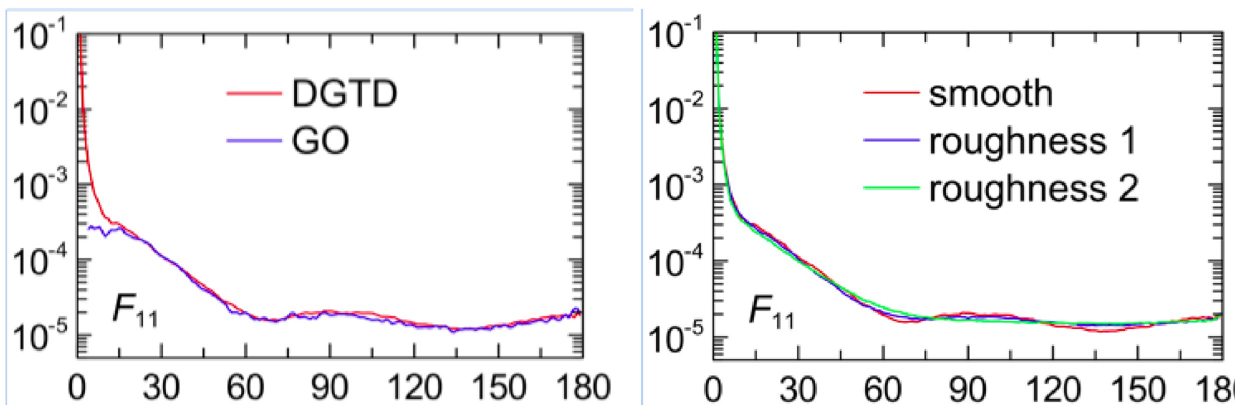


main result: size important, shape not so much

X=200:



TD-DG & DDA



good agreement, differences for imaginary part,

roughness only has some influence, but small

Biological photonic crystals

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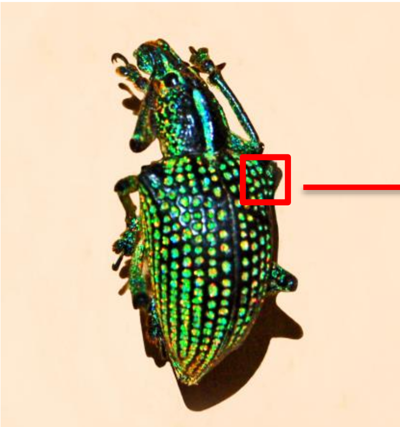
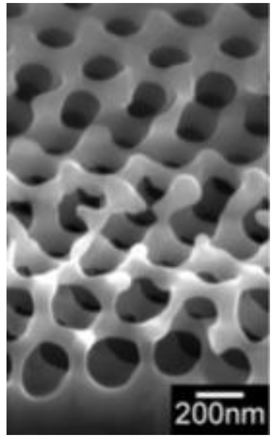
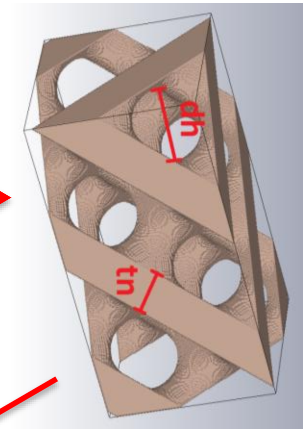
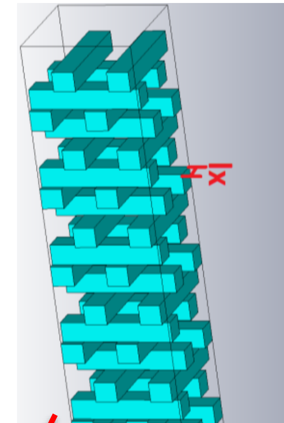
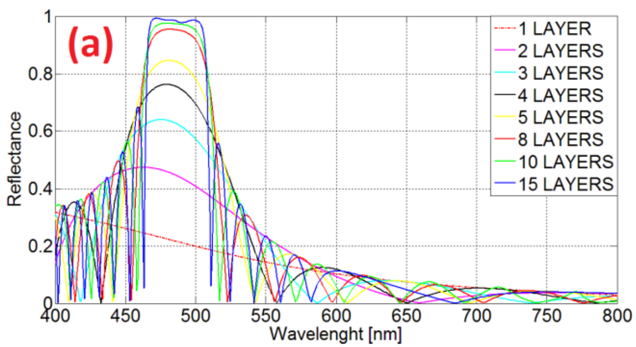
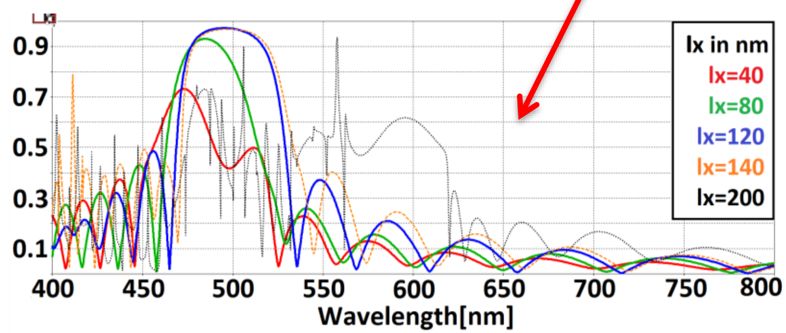








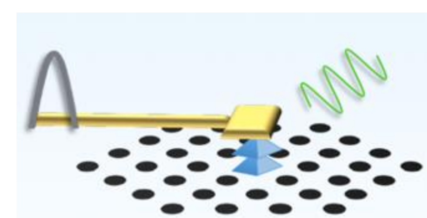




pronounced reflection band (with rotation of the circular polarization by multiple interference) ⇒ polarization filter

Biomimetic (i.e. related to nature, but technologically easier to realize) structure shows same behaviour

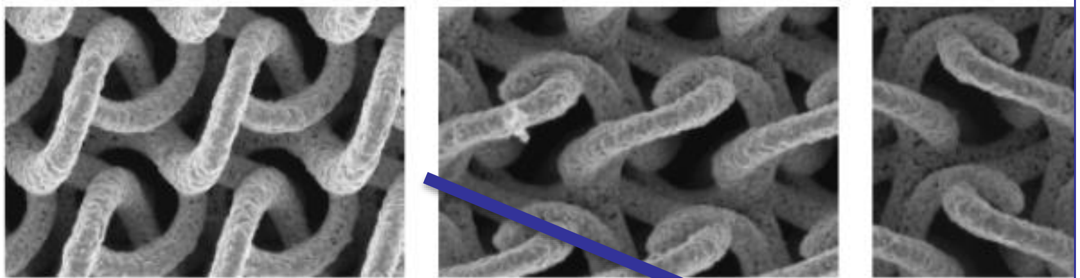
we also investigate artificial photonic crystals:



Cooperation with Xia Wu (UPB NW-C)

Bi-chiral photonic crystals

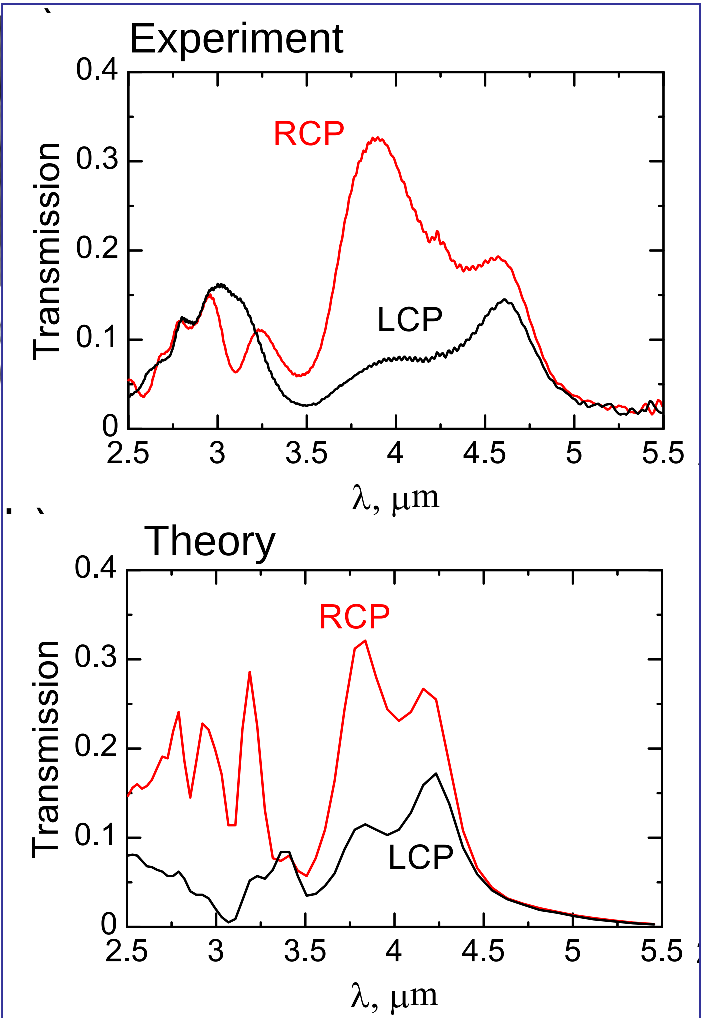
Triple interveaved helix array (H. Giessen/Stuttgart):



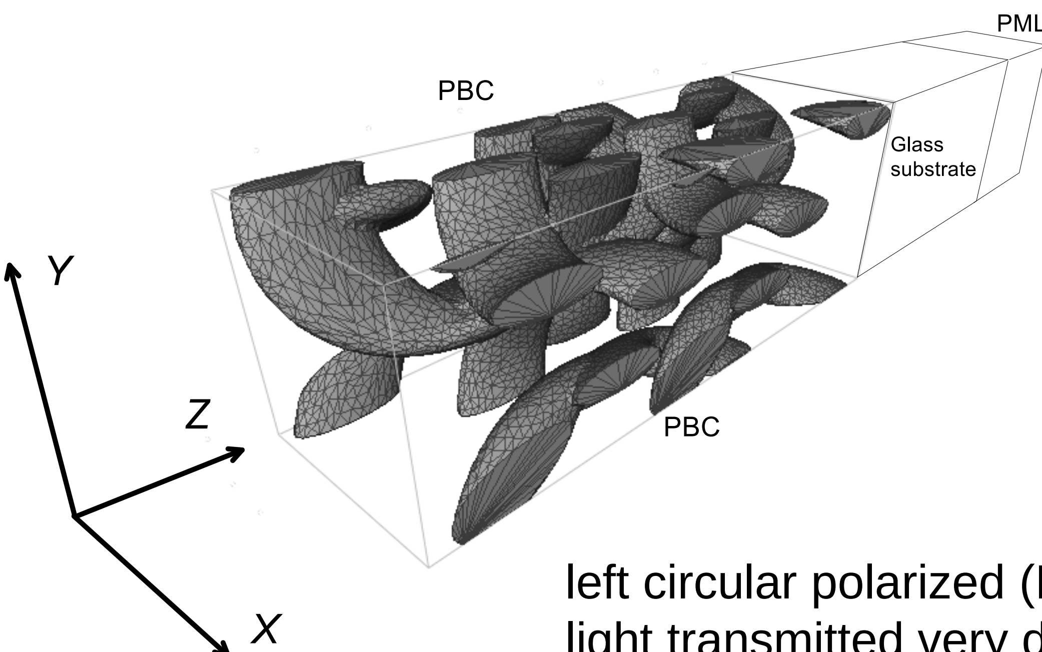
Left–handed corner
Left–handed helix

Left–handed corner
Right–handed helix

Right–hand…
Left–han…



Theory (Discontinuous Garlerkin):



left circular polarized (LCP) and right circular polarized (RCP) light transmitted very differently ⇒ **ultra thin polarizer**

HF circuits and antenna simulations

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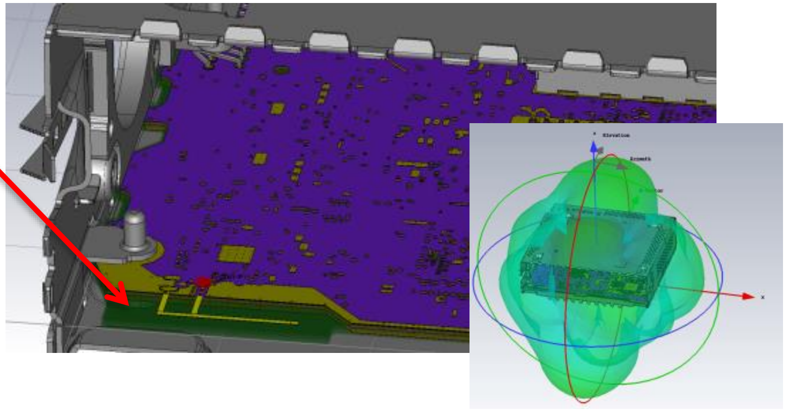
Simulation of a bluetooth antenna in a car radio/infotainment system

Consider electronics and housing

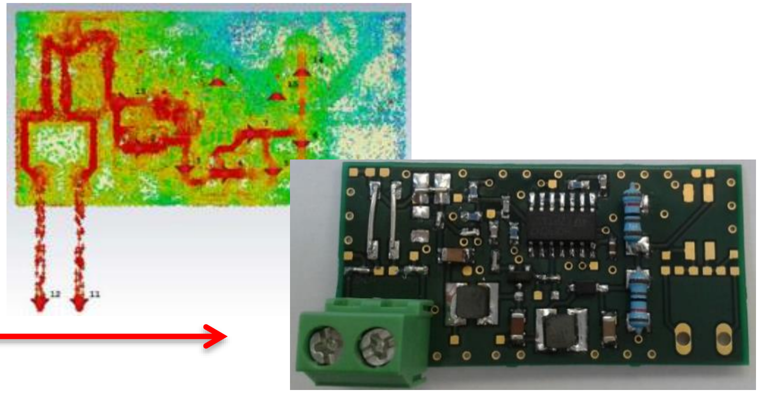
⇒ optimize radiation and EMC (Electromagnetic compatibility)



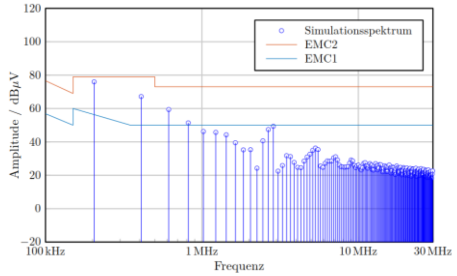
with Continental Automotive

EMC simulation of SEPIC (DC-DC)

Combination of Spice+Maxwell (with CST Studio)



- Verification of simulation method by measuring several designs
- Reduction of interference to fulfill EMC requirements



with Phoenix Contact

Thanks to

HPC: Paderborn Center for Parallel Computing

Christian Plessl and his team for acquiring and maintaining the PC2 systems, and cooperation/support on HPC programming

funding: Deutsche Forschungsgemeinschaft DFG
Sonderforschungsbereich TRR 142
CeOPP

And YOU for your attention!