New trends in material optimization

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Control of PDE

Benasque

26.08.2013

In the memory of Vicent Caselles

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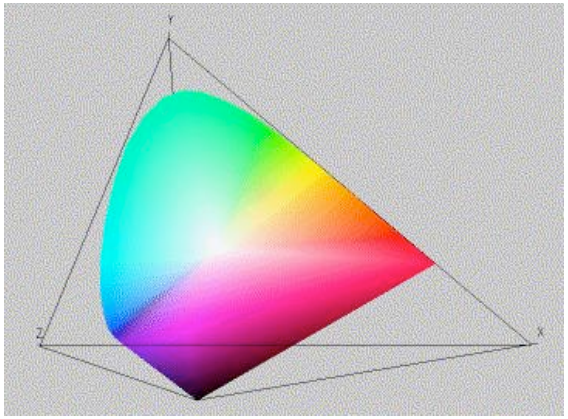
Department
MATHEMATIK

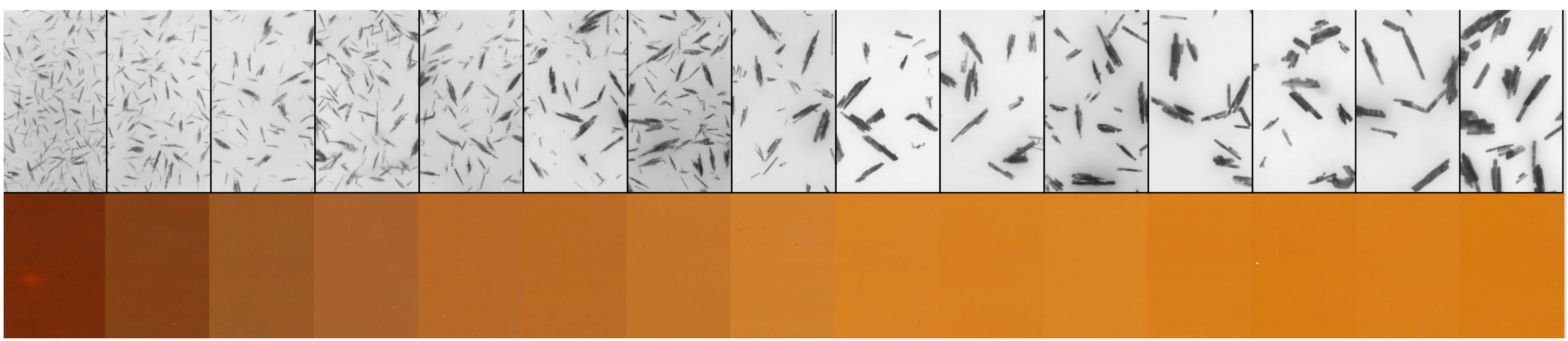
CONTINUOUS
OPTIMIZATION

Horseshoe metric and Cie-solid



Vicent Caselles' lecture in Benasque 2009 on the horseshoe metric paved the (my) way to optimization of optical properties

Colors strongly depend on particle shapes and their distributions see e.g. the values for a Goethite size distribution



Process chain

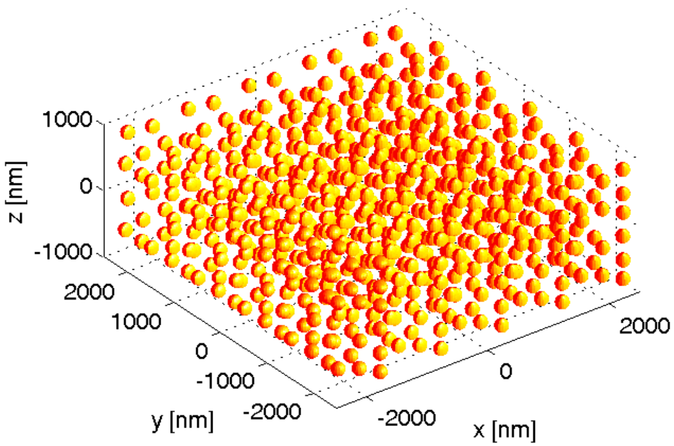
- Predefine a goal function in terms of Cie-values (spectral formulation)
- Construct the structure-porperty map (from the particle-shape to spectra)
- Optimize the shape with respect to that mapping (shape optimization)
- Produce particles with optimal shape (engng.: narrow size distribution)
- Immerse particles into a matrix material (particle laden flow)
- Apply thin film (avoid: delamitation, cracks)
- Verify optimal color properties

Mathematically this involves

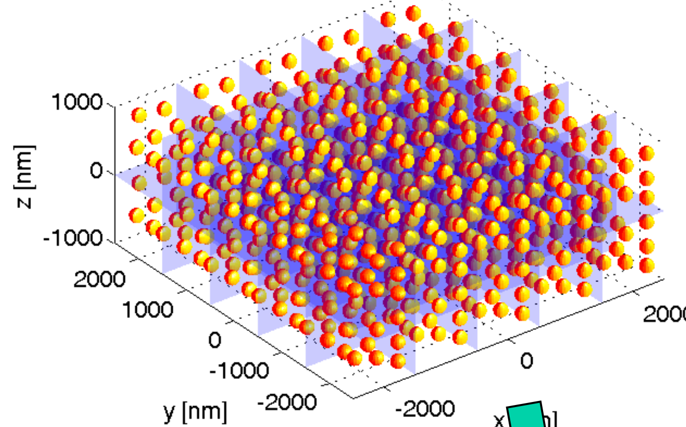
- constrained shape and topology optimization
- control-in-the-coefficients for nonlinear PDEs or VIs
- control the dynamics of particle-laden flows including dalamination and cracks

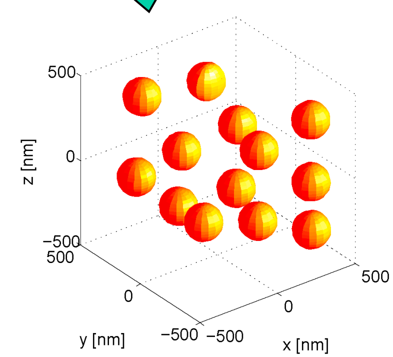
Pigment optimization in thin films via Mie-scattering theory

Pigment system

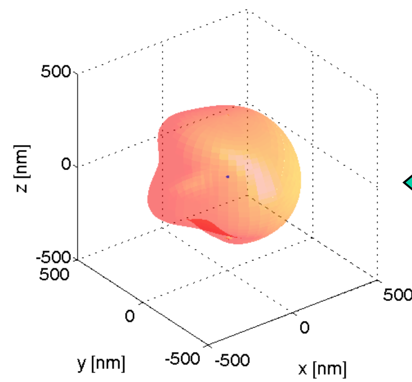


Split into smaller volumes

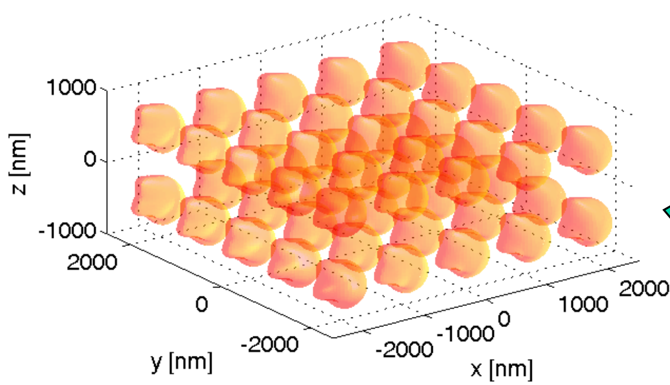




Compute volume element properties



Find single origin T-matrix



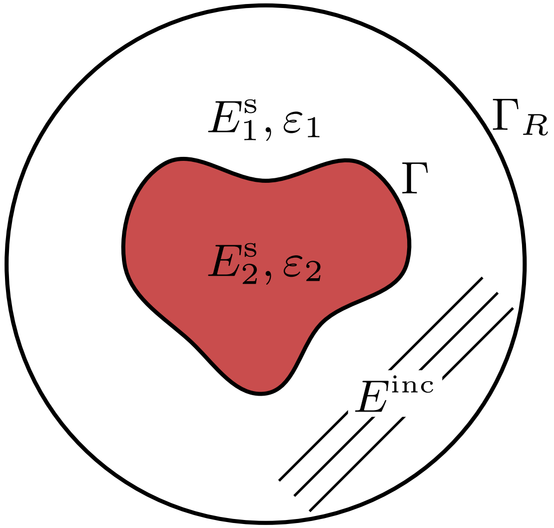
Compute the pigment system as interacting volume elements

Time harmonic Maxwell

curl-curl formulation of time-harmonic Maxwell's Equation:

scattering problem $E = E^{\mathbf{s}} + E^{\mathbf{inc}}$

$$\begin{aligned}
\operatorname{curl}\operatorname{curl} E_1^{\mathrm{s}} - \omega^2 \varepsilon_1 E_1^{\mathrm{s}} &= 0 && \Omega_1 \\
\operatorname{curl}\operatorname{curl} E_2^{\mathrm{s}} - \omega^2 \varepsilon_2 E_2^{\mathrm{s}} &= \omega^2(\varepsilon_2 - \varepsilon_1) E^{\mathrm{inc}} && \Omega_2 \\
[\operatorname{curl} E \times n] &= 0 && \Gamma \\
[E \times n] &= 0 && \Gamma \\
\operatorname{curl} E_1^{\mathrm{s}} \times n_1 - i\omega E_{T,1}^{\mathrm{s}} &= 0 && \Gamma_R
\end{aligned}$$



with $E_1^{\mathrm{s}}, E_2^{\mathrm{s}}$ scattered fields, E^{inc} incident field,
$\varepsilon_1 \in \mathbb{R}$, $\varepsilon_2 \in \mathbb{C}$ relative permittivity

Energies

Energy decomposition

$$W_{\text{abs}} = \underbrace{W_{\text{inc}}}_{\equiv 0} + W_{\text{ext}} - W_{\text{sca}}$$

Absorption cross section

$$\begin{aligned} W_{\text{abs}}(\Omega_2) &= -\int_{\partial F} S \cdot n \\ &= \frac{\omega}{2}\,\text{Im}(\varepsilon_2) \int_{\Omega_2} |E^{\text{s}}|^2 + 2\,\text{Re}(E^{\text{s}} \cdot \bar{E}^{\text{inc}}) + |E^{\text{inc}}|^2 \; \text{d}x \end{aligned}$$

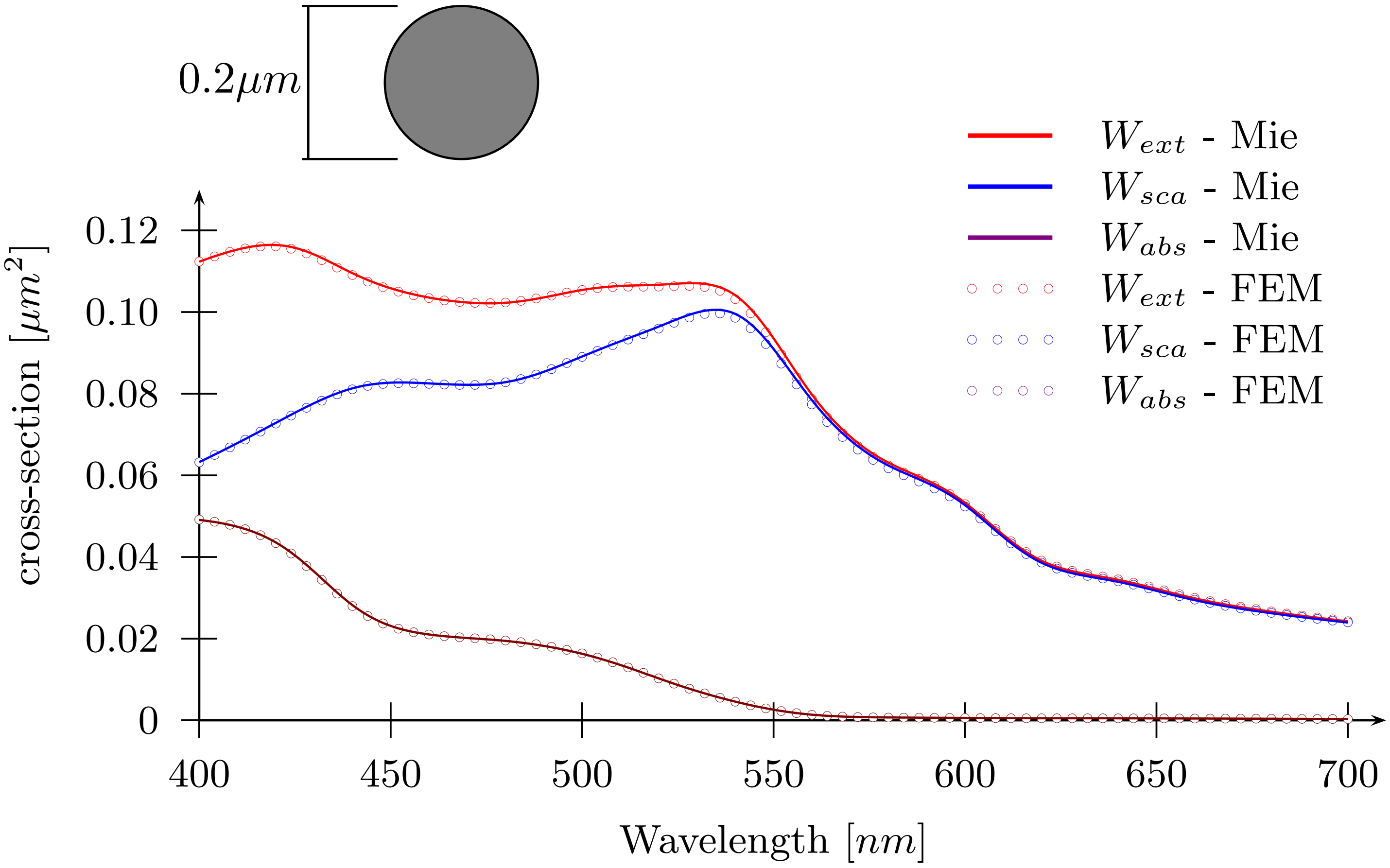
Extinction cross section

$$\begin{aligned} W_{\text{ext}}(\Omega_2) &= -\int_{\partial F} S^{\text{ext}} \cdot n \\ &= \frac{\omega}{2} \int_{\Omega_2} \text{Im}\Big((\varepsilon_2 - \varepsilon_1)\big(E^{\text{inc}} \cdot \bar{E}^{\text{s}}\big)\Big) - \text{Im}(\varepsilon_2)\; \text{d}x \end{aligned}$$

Code validation vs. Mie

Solution of FEM compared to Mie theory solution:

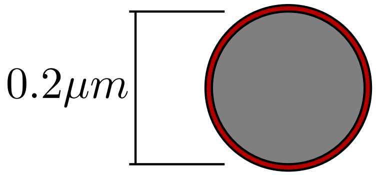
Goethite sphere with 200nm diameter in H_2O

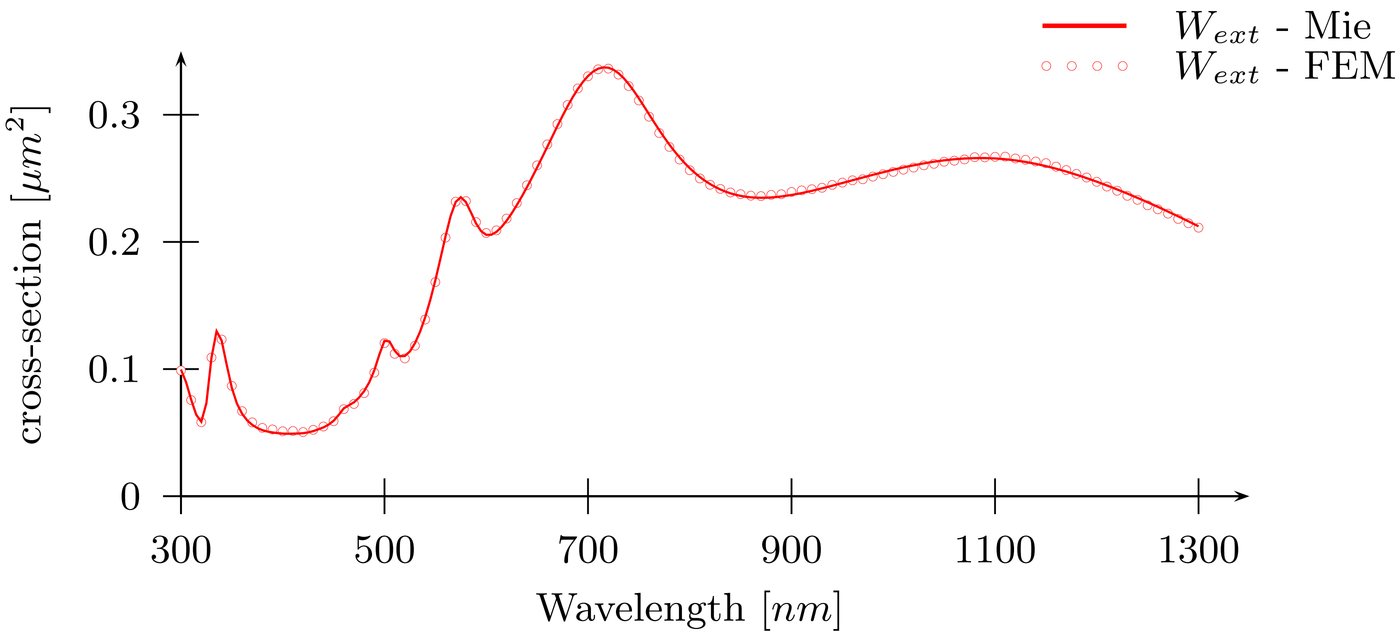


Code validation vs. Mie

Solution of FEM compared to Mie theory solution:

Silica sphere with 200nm diameter coated with a 15nm silver shell

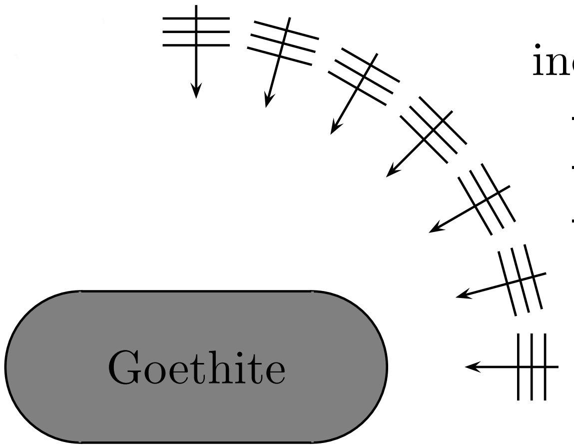




Szenarios

Problem setting

Goethite nanorods in H_2O
- different length / width ratios
- equivalent volume

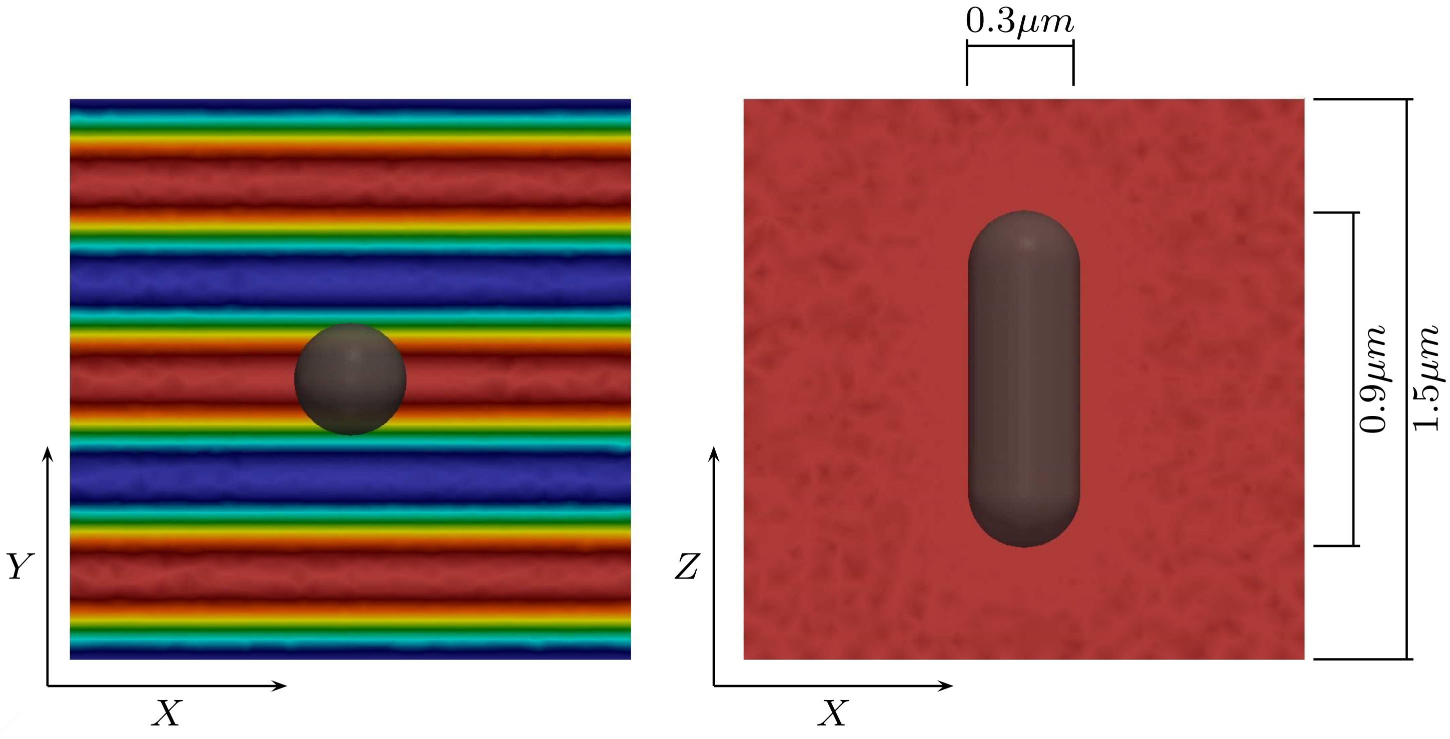


incident waves
- 96 different directions
- 4 polarizations each
- cross sections averaged

Optical properties of nanorods

3D FEM to simulate time-harmonic electromagnetic fields:

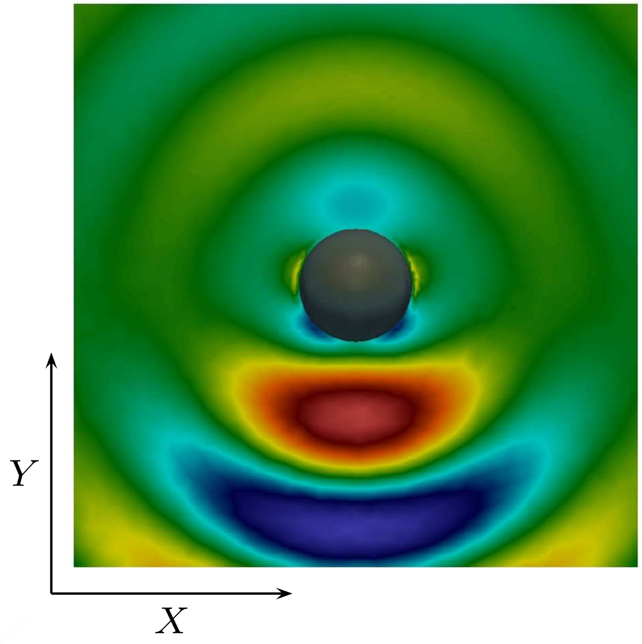
X-component of incident field $(\lambda = 600nm)$

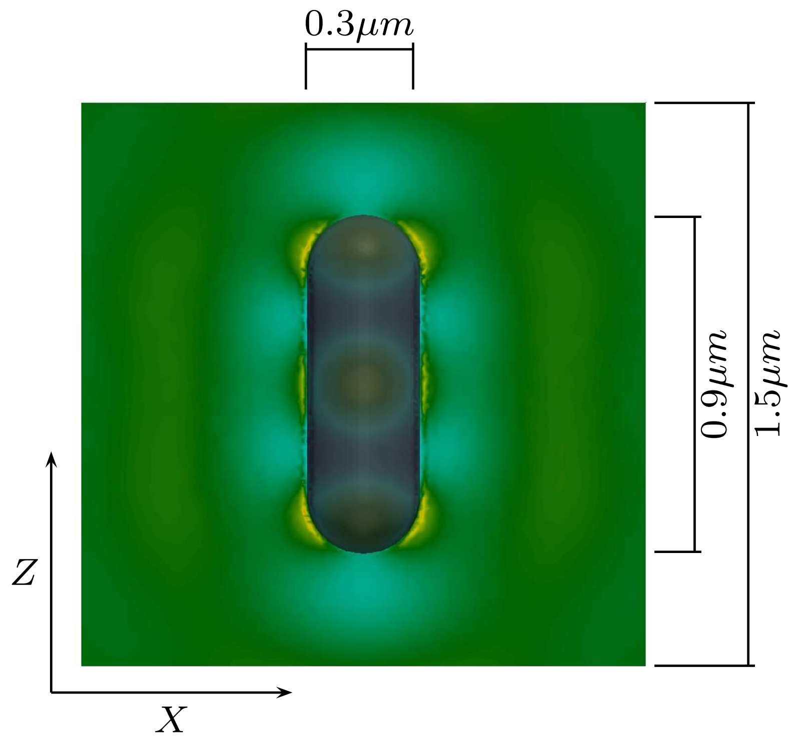


FEM Simulation

3D FEM to simulate time-harmonic electromagnetic fields:

X-component of scattered field ($\lambda = 600nm$)

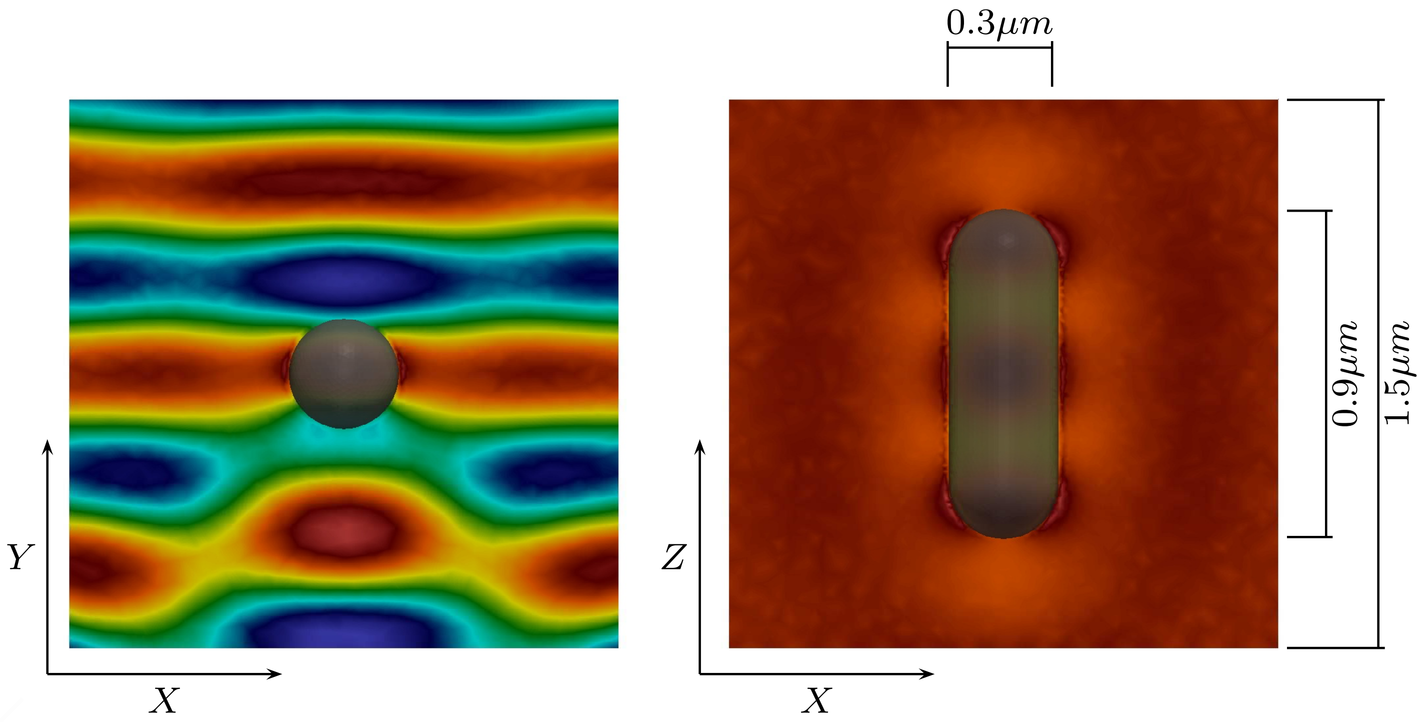




FEM Simulation

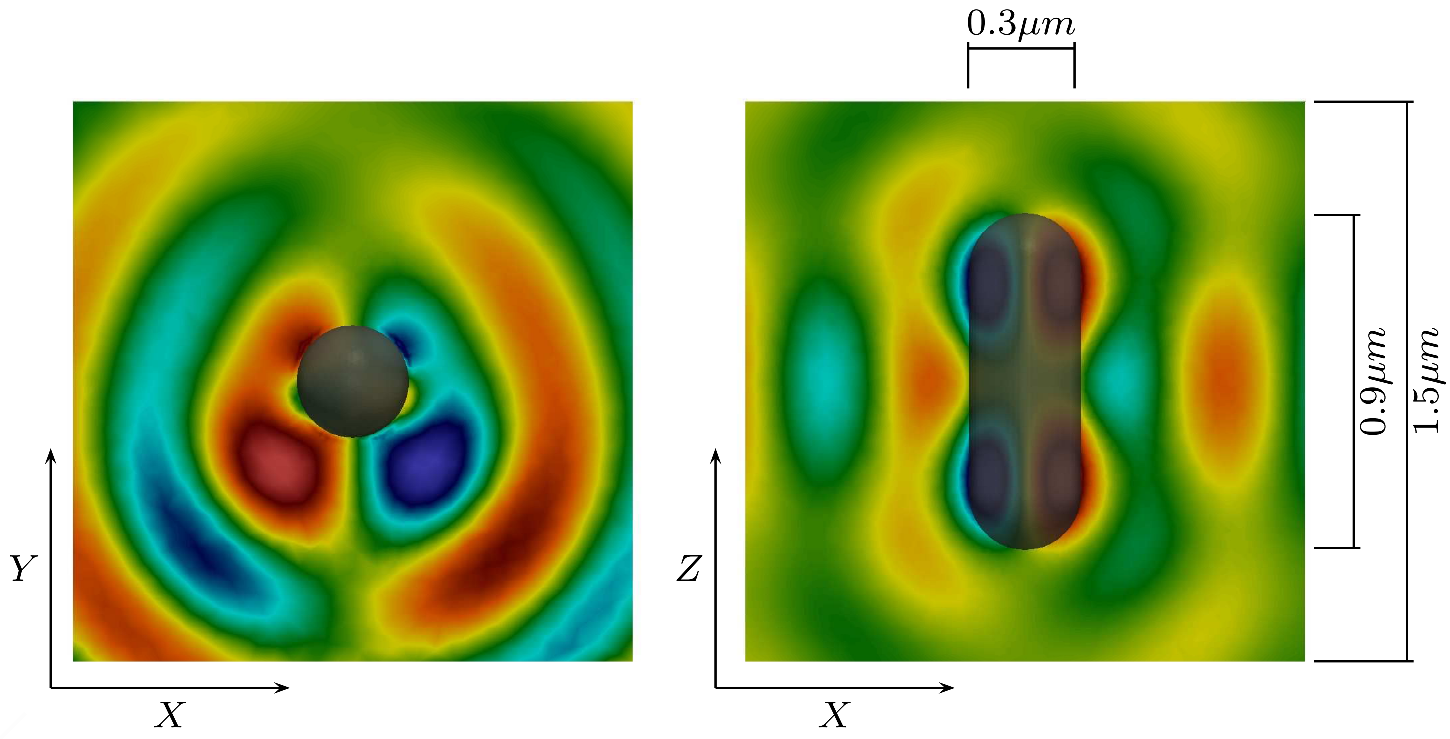
3D FEM to simulate time-harmonic electromagnetic fields:

X-component of total field $(\lambda = 600nm)$



3D FEM to simulate time-harmonic electromagnetic fields:

Z-component of scattered field ($\lambda = 600nm$)

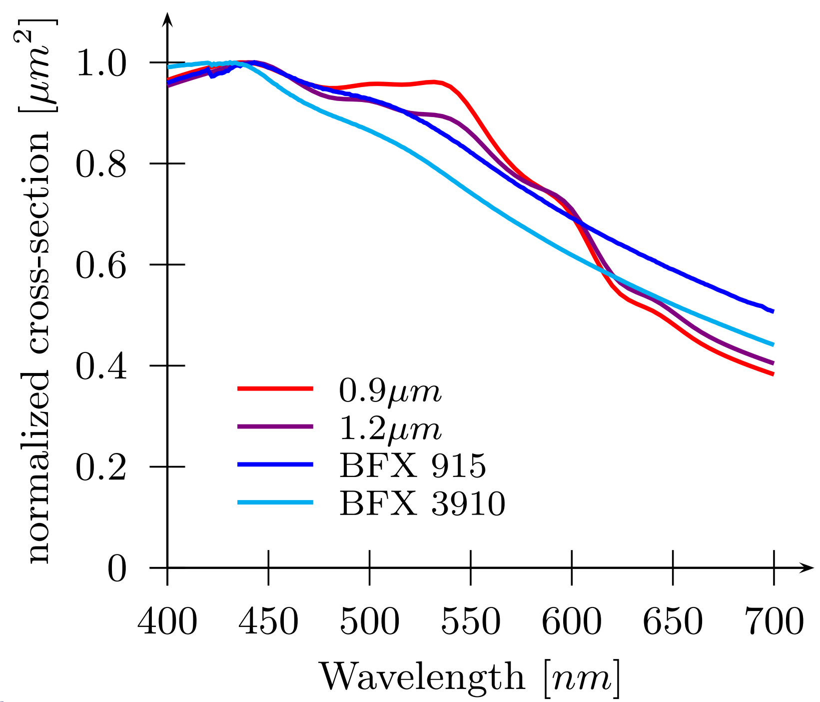


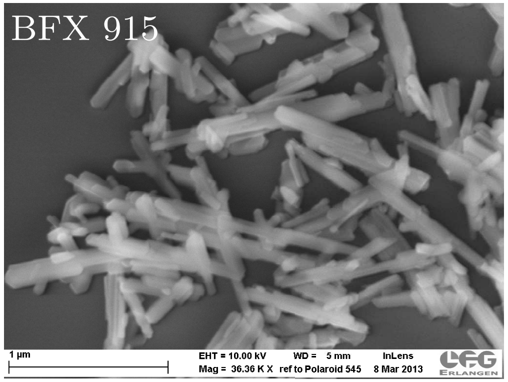
Validation against experiment

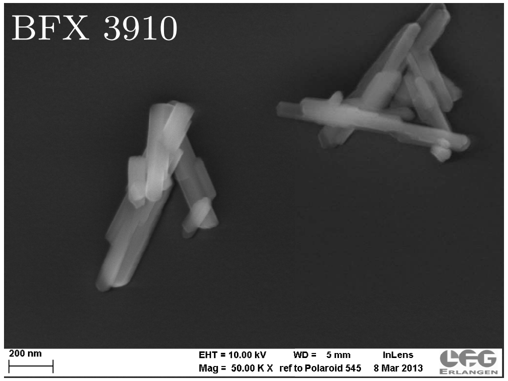
comparison: Simulation vs. Experiment

Simulation: Goethite nanorod with 150nm diameter
and 0.9 μm / 1.2 μm length

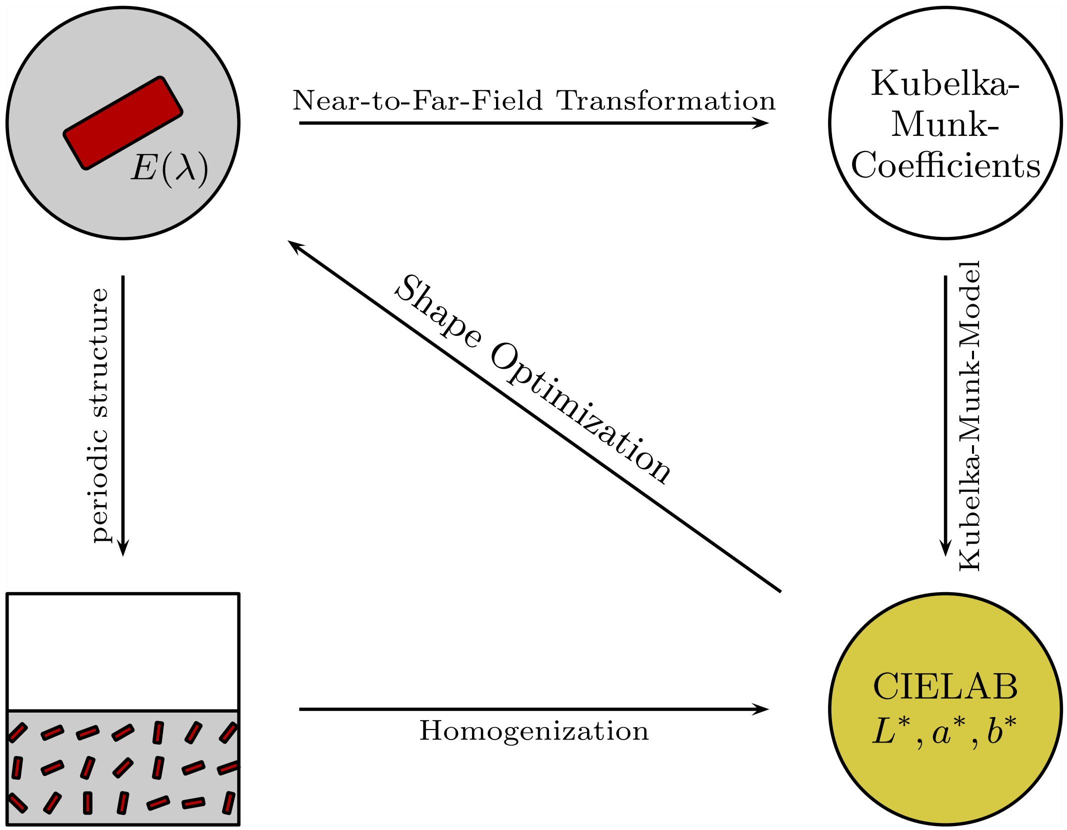
Experiment: Absorbance of two commercial pigments dispersed in water
at very low concentration





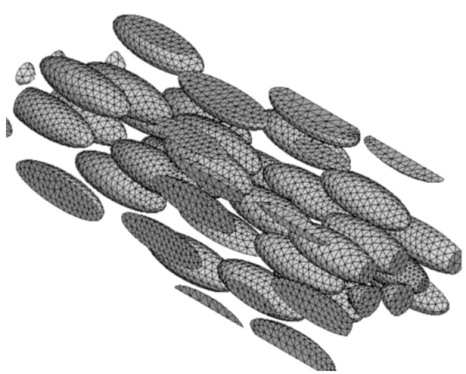


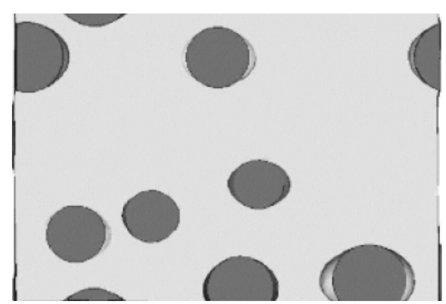
New trends in material optimization: From color to shape and material



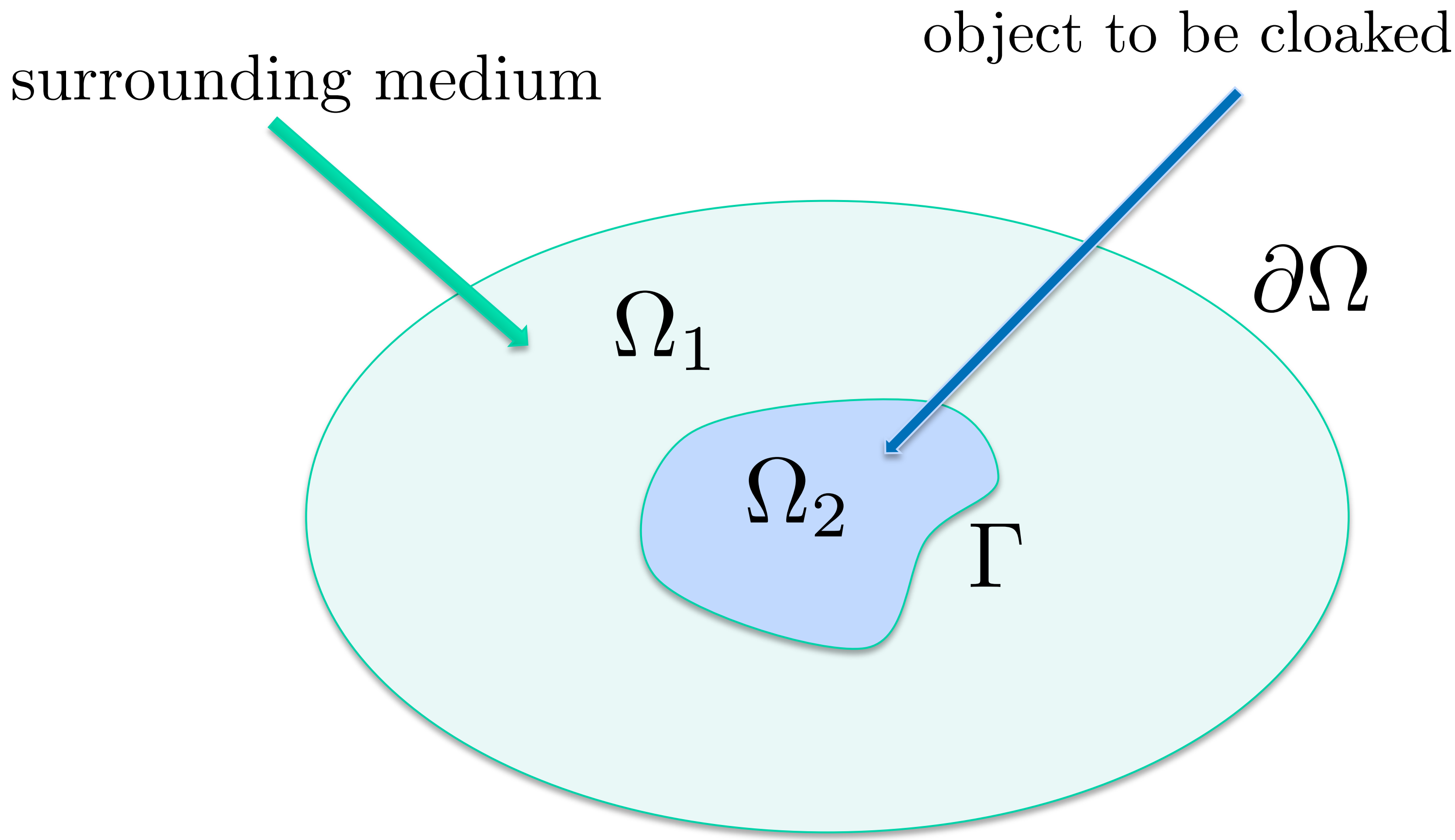
Cooperations w.r.t. material optimization

- A. Novotny, G. Perla-Menzala and J. Sokolowski (piezos, shape)
- S. A. Nazarov, F. Schury, M. Stingl (topology optimization for piezos)
- A. Khludnev (Griffith cracks, inlcusions)
- M. Prechtel, P. Steinmann, M. Stingl (cohesive cracks, inclusions)
- S.A. Nazarov, A. Slutskij (asymptotic analysis, thin-domains)
- E. Bänsch, M. Kaltenbacher, F. Wein, F. Schury, M. Stingl (SIMP, TopGrad)
- P. Kogut, M. Stingl, F. Seifrt (damage, cloaking)
- J. Haslinger, M. Kocvara, E. Rohan, M. Stingl, (metamaterials. homogenization, FMO)
- C. Le Bris, V. Ehrlacher, Stingl (non-periodic homogenization and optimization)





Cloaking: geometry setup



Time-harmonic Maxwell ctd.

Let us assume for a while, that the material is homogeneous, i.e. (ϵ, μ, σ) are constants. Then either $\boldsymbol{E}$, or $\boldsymbol{H}$ can be eliminated, so that the Helmholtz equations hold

$$\nabla^2 \boldsymbol{E} + \kappa^2 \boldsymbol{E} = \epsilon^{-1} \nabla \rho - \mathrm{i}\omega\mu \boldsymbol{J}_e , \quad \nabla \cdot \boldsymbol{E} = \rho/\epsilon ,$$
$$\nabla^2 \boldsymbol{H} + \kappa^2 \boldsymbol{H} = -\nabla \times \boldsymbol{J}_e , \quad \nabla \cdot \boldsymbol{H} = 0 ,$$

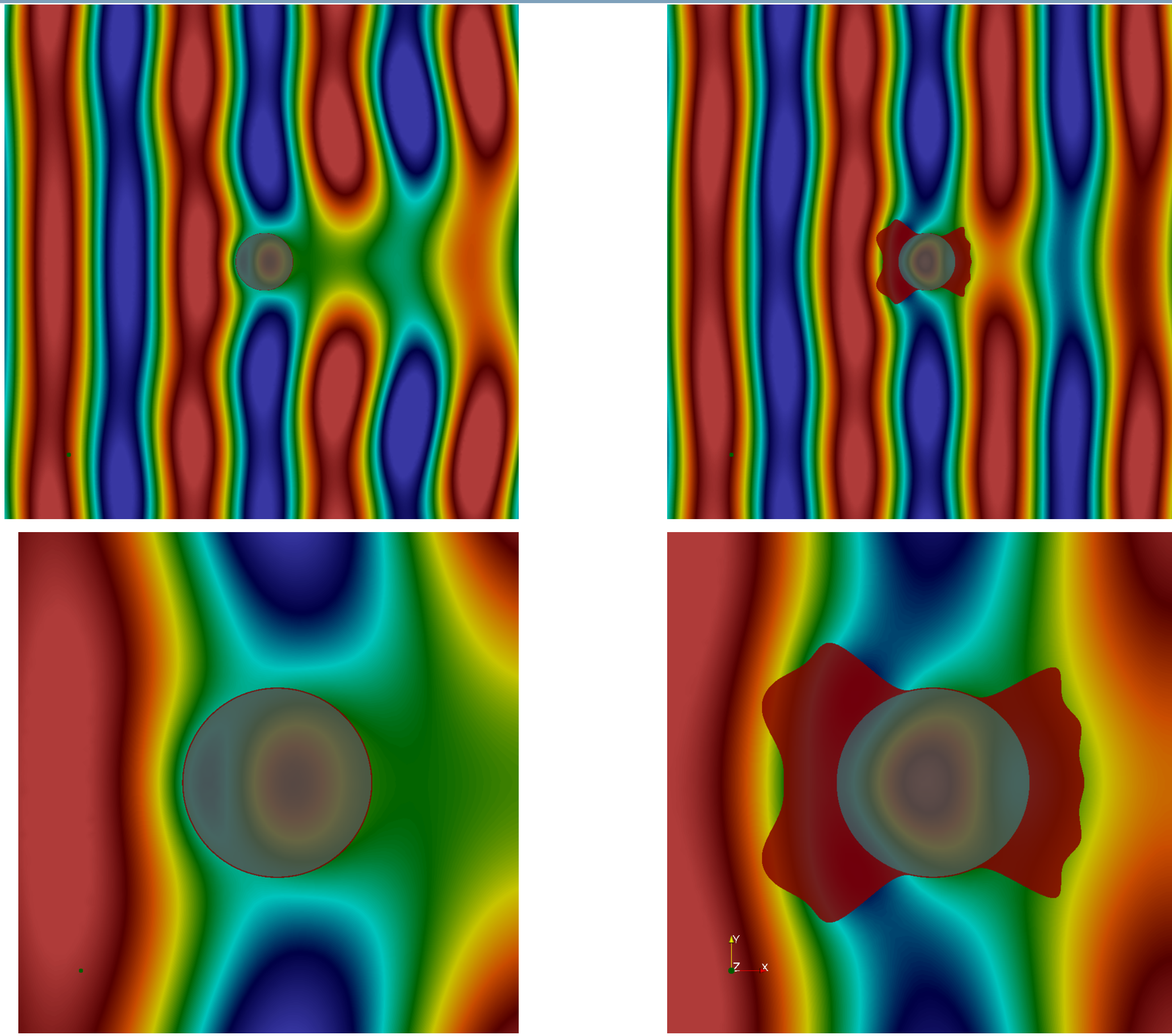
where κ is the wave number characterized by the material:

$$\kappa^2 = \omega^2 \mu \beta = \omega^2 \mu (\epsilon + \mathrm{i}\sigma/\omega) .$$

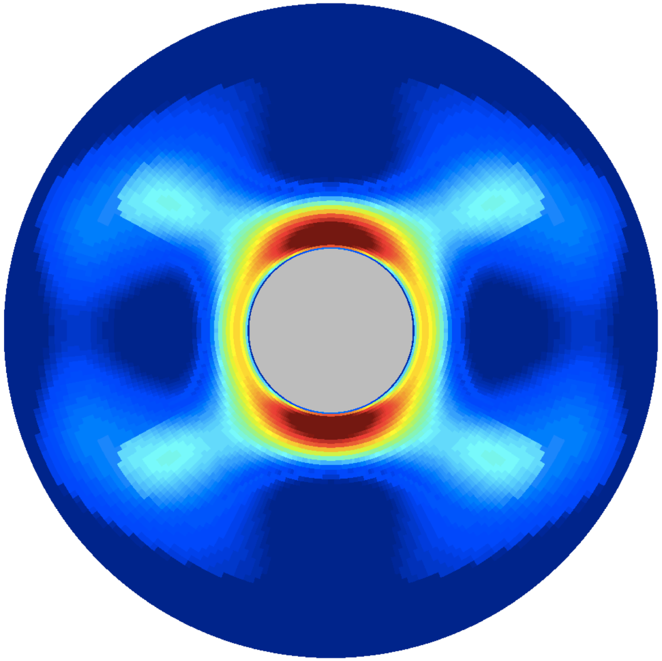
Results for 2-D shape optimization

wave length λ	500nm
particle	
radius	100nm
material	Hematite (Fe_2O_3, $n(\lambda) = 2.971 + 0.317i$)
coating	
bounds:	100 - 200nm
refr. index:	$n = 2$
incident wave	plane wave x-dir., z-pol.
Num.	
DoFs	ca. 400.000
basis	P2-Lagrange
Objective func	zero tracking of scattered field
Reduction:	70%

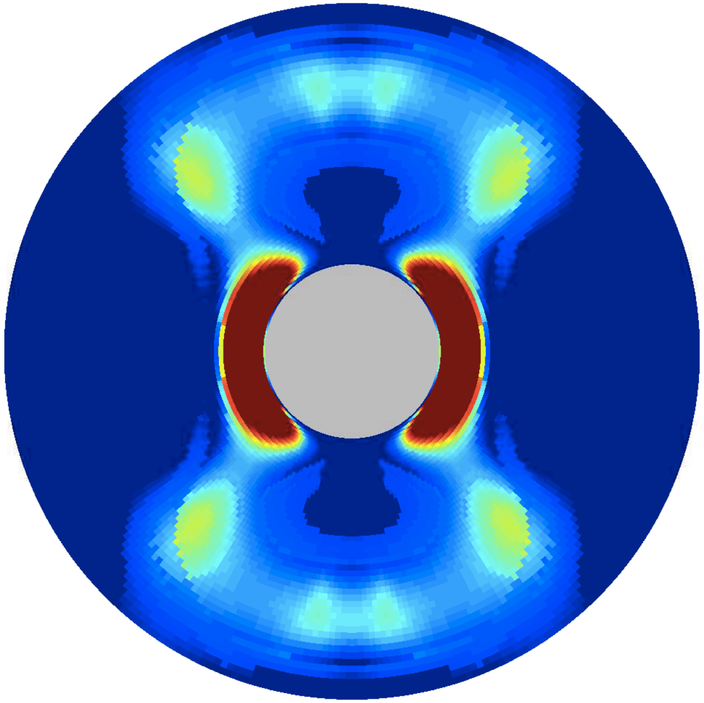
2-D Shape optimization



Optimal design for multiple directions (SIMP)

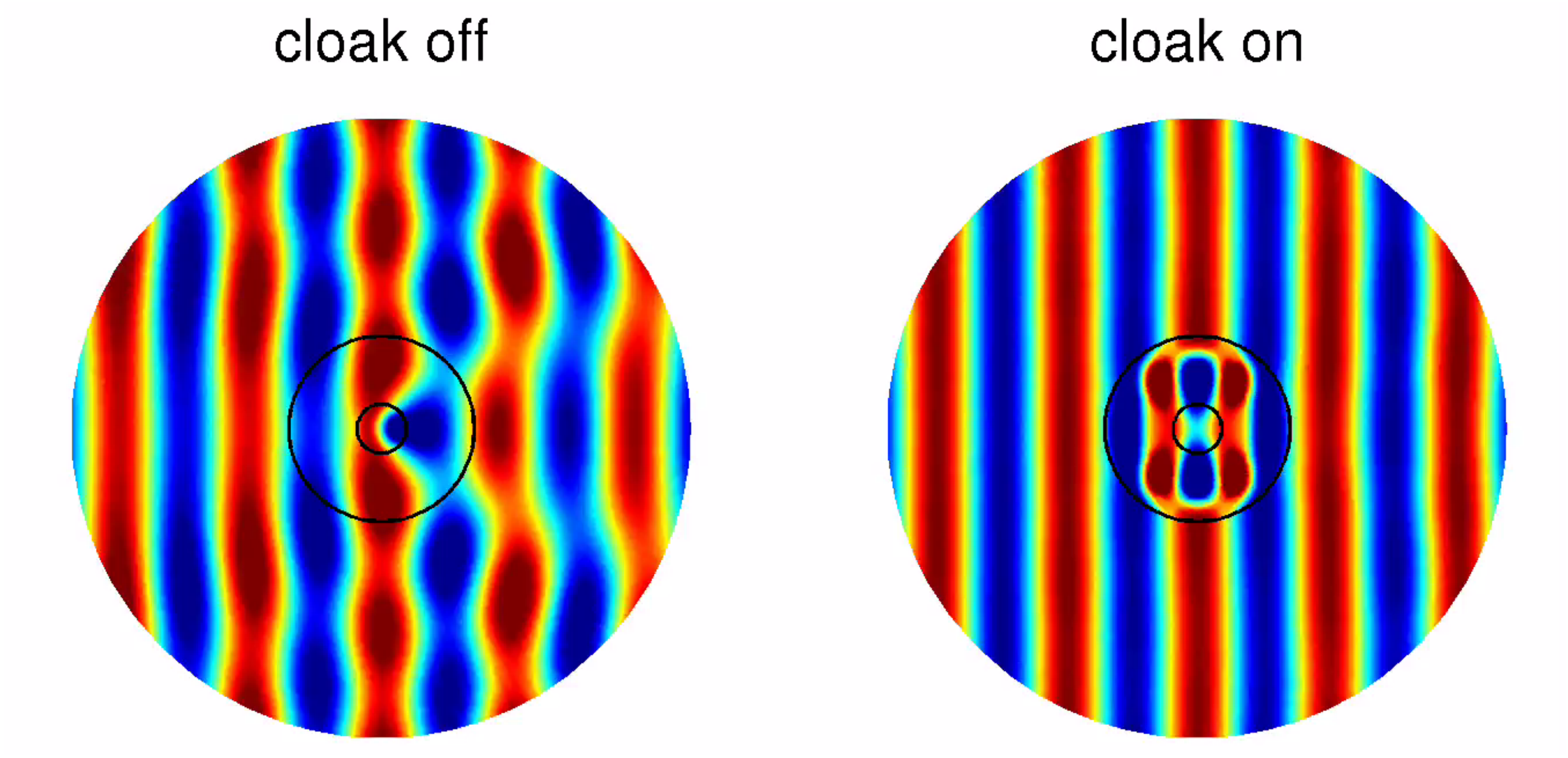


Optimal design for 3 directions, $\Sigma = \{-1/4\pi, 0, 1/4\pi\}$



Optimal design for 4 directions, $\Sigma = \{-1/2\pi, -1/3\pi, 1/3\pi, 1/2\pi\}$

‚Exact‘ cloaking for one frequency



Computations by F. Seifrt

3-D shape gradient

- primal problem:

$$\mathrm{curl}\,\frac{1}{\mu_r}\,\mathrm{curl}\,E_s - \kappa^2\epsilon_r E_s = \mathrm{curl}(\frac{1}{\mu_r^b} - \frac{1}{\mu_r})\,\mathrm{curl}\,E_i - \kappa^2(\epsilon_r^b - \epsilon_r)E_i =: f$$

- objective functional:

$$J(\Omega, E_s) = \frac{1}{2}\int_S |E_s|^2\,\mathrm{d}x$$

- notation:

$$u_T = n \times (u \times n)$$

$$(\cdot,\cdot)_\Omega = \sum(\cdot,\cdot)_{\Omega_i} \qquad (\cdot,\cdot)_\Gamma = \sum(\cdot,\cdot)_{\Gamma_i}$$

$$\langle u, v\rangle_B = \frac{1}{2}(u,v)_B + \frac{1}{2}(v,u)_B$$

- partial integration:

$$\int_B \mathrm{curl}(\mathrm{curl}\,u)\cdot v\,\mathrm{d}x = \int_B \mathrm{curl}\,u\cdot\mathrm{curl}\,v\,\mathrm{d}x - \int_{\partial B}((\mathrm{curl}\,u)\times n)\cdot v_T\,\mathrm{d}\omega$$

- weak formulation:

$$(\mu^{-1}\,\mathrm{curl}\,E_s, \mathrm{curl}\,\phi)_\Omega - (\mu^{-1}(\mathrm{curl}\,E_s)\times n, \phi_T)_\Gamma - (\omega^2\epsilon E_s, \phi)_\Omega = (f,\phi)_\Omega$$

3-D shape gradient

- Lagrange functional: $(v, q \in H(\mathrm{curl}, \mathbb{R}^3))$:

$$L(\Omega, v, q) = J(\Omega, v) + \langle \mu^{-1} \,\mathrm{curl}\, v, \mathrm{curl}\, q \rangle_\Omega - \langle \omega^2 \epsilon v, q \rangle_\Omega - \langle f, q \rangle_\Omega \\ - \langle \mu^{-1} (\mathrm{curl}\, v) \times n, q_T \rangle_\Gamma - \langle v_T, \bar{\mu}^{-1} (\mathrm{curl}\, q) \times n \rangle_\Gamma$$

- adjoint system:

$$(\bar{\mu}^{-1} \,\mathrm{curl}\, W_s, \mathrm{curl}\, \phi)_\Omega - (\mu^{-1} (\mathrm{curl}\, W_s) \times n, \phi_T)_\Gamma - (\omega^2 \epsilon W_s, \phi)_\Omega = -(E_s, \phi)_\Omega$$

- shape gradient:

$$\mathrm{d}J(\Omega; V) = \langle \mu^{-1} \,\mathrm{curl}\, E_s, \mathrm{curl}\, W_s (V \cdot n) \rangle_\Gamma - \langle \omega^2 \epsilon E_s, W_s (V \cdot n) \rangle_\Gamma - \langle f, W_s (V \cdot n) \rangle_\Gamma$$

3-D shape gradient

- notation:

$$\Gamma_{i,j} = \Gamma_i \cap \Gamma_j$$

- summation formula:

$$\sum_{i,j} \langle A_i, B_i(V \cdot n_i) \rangle_{\Gamma_{i,j}} = \sum_{i<j} \langle A_i, B_i(V \cdot n_i) \rangle_{\Gamma_{i,j}} - \langle A_j, B_j(V \cdot n_i) \rangle_{\Gamma_{i,j}} = \sum_{i<j} \langle [A \cdot \bar{B}]_{i,j}, (V \cdot n_i) \rangle_{\Gamma_{i,j}}$$

- shape gradient:

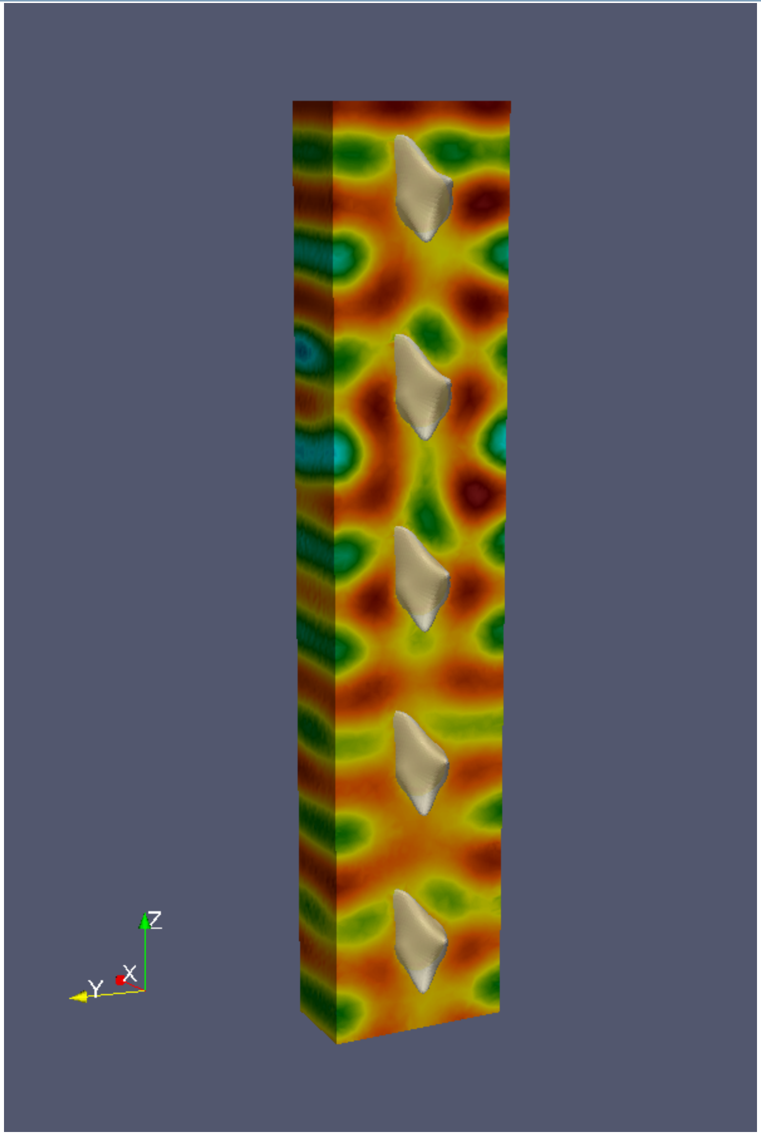
$$\begin{aligned} \mathrm{d}J(\Omega; V) &= \sum_{i<j} \Big\langle [\mu^{-1} \operatorname{curl} E_s \cdot \operatorname{curl} \bar{W}_s]_{i,j} - [\omega^2 \epsilon E_s \cdot \bar{W}_s]_{i,j} - [f \cdot \bar{W}_s]_{i,j}, (V \cdot n_i) \Big\rangle_{\Gamma_{i,j}} \\ &= \sum_{i<j} \Big(\mathrm{Re}\big([\mu^{-1} \operatorname{curl} E_s \cdot \operatorname{curl} \bar{W}_s]_{i,j} - [\omega^2 \epsilon E_s \cdot \bar{W}_s]_{i,j} - [f \cdot \bar{W}_s]_{i,j} \big), (V \cdot n_i) \Big)_{\Gamma_{i,j}} \end{aligned}$$

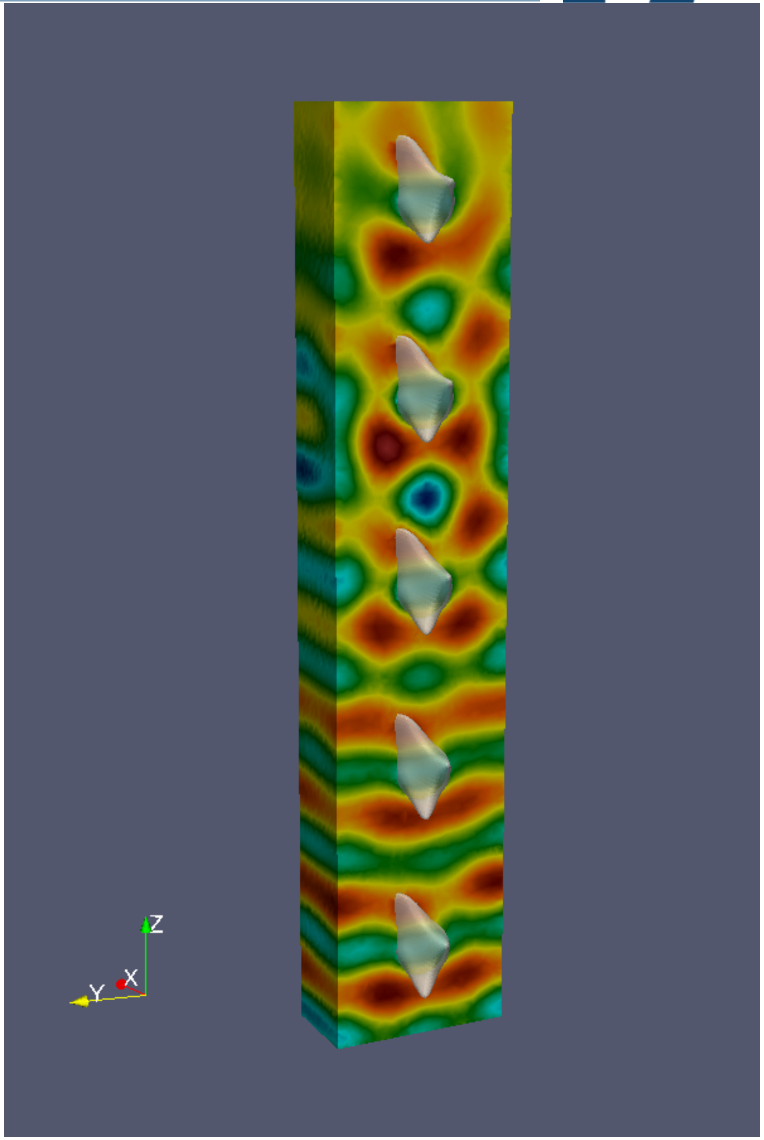
3-D forward simulations

material: Hematite (Fe_2O_3)
incident wave: plane wave $-z$-dir, x-pol.

particle size	wavelength	PML	periodicity
500nm	500nm	z	xy
500nm	500nm	xyz	-
500nm	500nm	z	xy
300nm	500nm	xyz	-

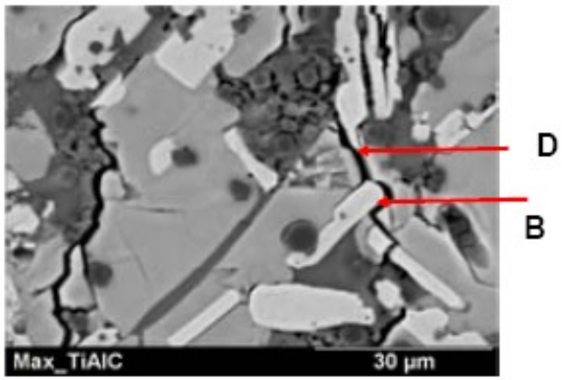
Different shapes: not yet optimized

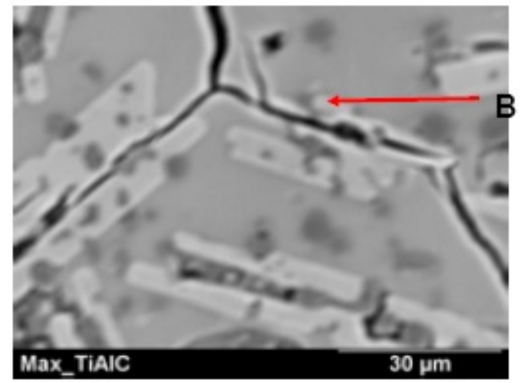


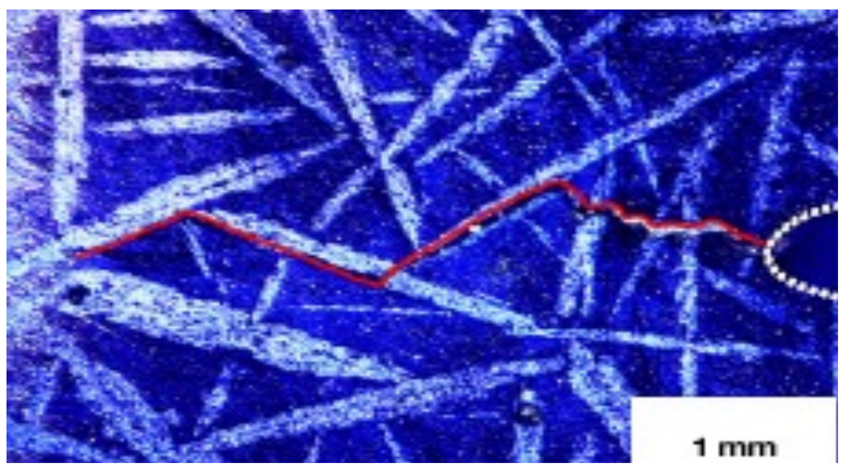


New trends in material optimization: control of cracks and damage

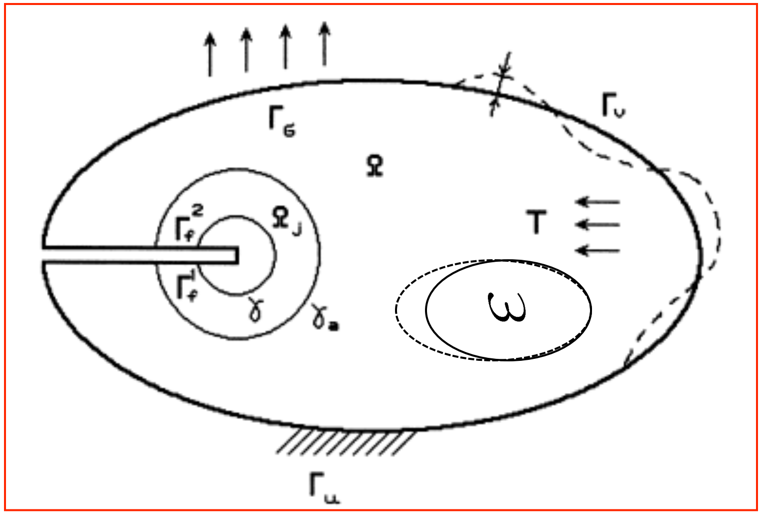
Crack propagation behavior in the $Ti_3AlC_2/TiAl_3$-composite

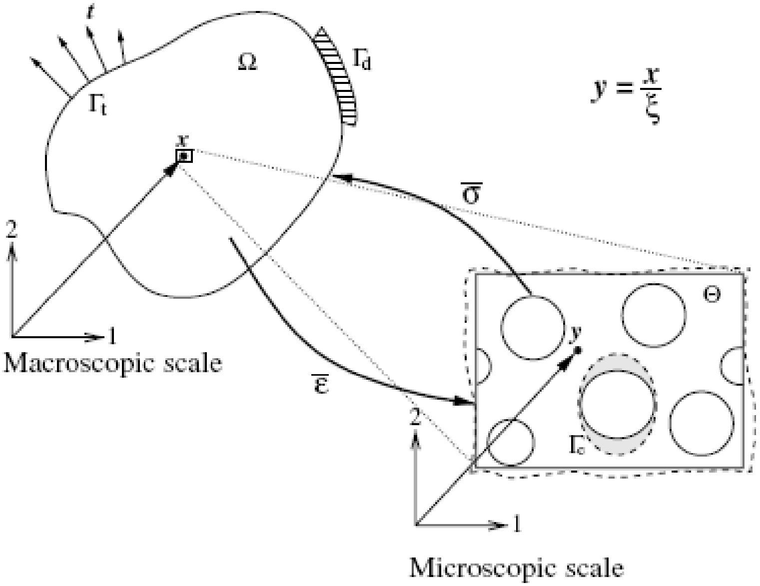






Can we control the evolution of damage and cracks?





- boundary forces or distributed forces (see Münch et.al. 2006)
- boundary variations along a part of the boundary? (see Saurin 2006)
- variation of material or shape of inclusions?

  (with Prechtel, Steinmann, Khludnev 2010)
- ,inverse' homogenization? (with Kogut and Stingl)

Setup for Griffith theory

$$\begin{aligned} -\text{div}\,\sigma = f \quad &\text{in} \quad \Omega_\gamma, \\ \sigma - A\varepsilon(u) = 0 \quad &\text{in} \quad \Omega_\gamma, \\ u = 0 \quad &\text{on} \quad \Gamma, \end{aligned}$$

$$[u_\nu] \geq 0,\ \sigma_\nu^\pm \leq 0,\ [\sigma_\nu] = 0,\ \sigma_\tau^\pm = 0,\ \sigma_\nu [u_\nu] = 0 \text{ on } \gamma.$$

- $\Omega_\gamma = \Omega \backslash \gamma$ domain without crack
- $[\cdot] = (\cdot)|_{\gamma^+} - (\cdot)|_{\gamma^-}$ jump along γ
- strain tensor $e_{ij}(u(x)) = \frac{1}{2}(\frac{\partial u_i(x)}{\partial x_j} + \frac{\partial u_j(x)}{\partial x_i})$, for $i, j = 1, 2$
- symmetric elasticity tensor $A_{ijkl} \in L^\infty$, $i, j, k, l = 1, \ldots, 2$
- stress tensor $\sigma_{ij} = A_{ijkl} e_{kl}$ (Hooke's law)

Extension for Barenblat theory

We consider the potential energy $P(u;\Omega_0)$ and the surface energy $S(u;\Omega_0)$ associated wirh the crack Γ_C

$$P(u;\Omega_0) := \frac{1}{2}\int_{\Omega_0} \sigma(u)\epsilon(u)dx - \int_{\Gamma_N} fuda$$

$$S(u;\Omega_0) := \int_{\Gamma_C} G([u]\nu)da$$

where $G \in C^{0,1}(\mathbf{R})$ is a density of the surface energy, $G > 0$. Morevover, we consider the non-penetration condition

$$[u]\nu \geq \text{ on } \quad \Gamma_C$$

i.e. we require $u \in K$ where K is given by

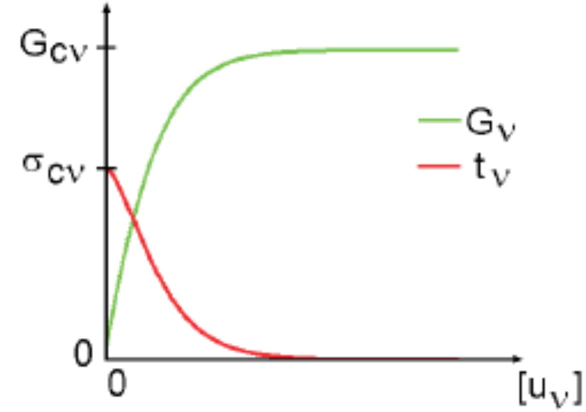
$$K = \{u \in H^1(\Omega_0) | u = 0 \text{ on } \Gamma_D, \quad [u]\nu \geq 0 \text{ on } \Gamma_C\}$$

A nonconvex minimization problem

We wish to minimize $T(\cdot;\Omega_0) := P(u;\Omega_0) + S(u;\Omega_0)$
over admissible displacements $u \in K$:

$$\min T(u;\Omega_0) \text{ s.t. } u \in K$$

In the Griffith case *G* is a constant
and the minimization problem amounts
to minimizing the potential energy *P*.
One can show existence of a solution using
w-*lsc* of *T* , w-closedness of *K* and coercivity
of *T.*



For *G=const,* this is classic! See e.g. Khludnev's book 2000
For normal cohesiveness (incl. Nonpenetration):
see Kovtunenko ZAMM 2005

Control the fracture energy

goal: maximization of fracture energy J:

$$\max_{\omega_1,\omega_2,\ldots,\omega_N\in\mathcal{E}} J(u) \qquad \text{s.t.}$$

with

$$J(u) := \int_\gamma G_\nu([u_\nu])\,da + \int_\gamma G_\tau([u_\tau])\,da$$

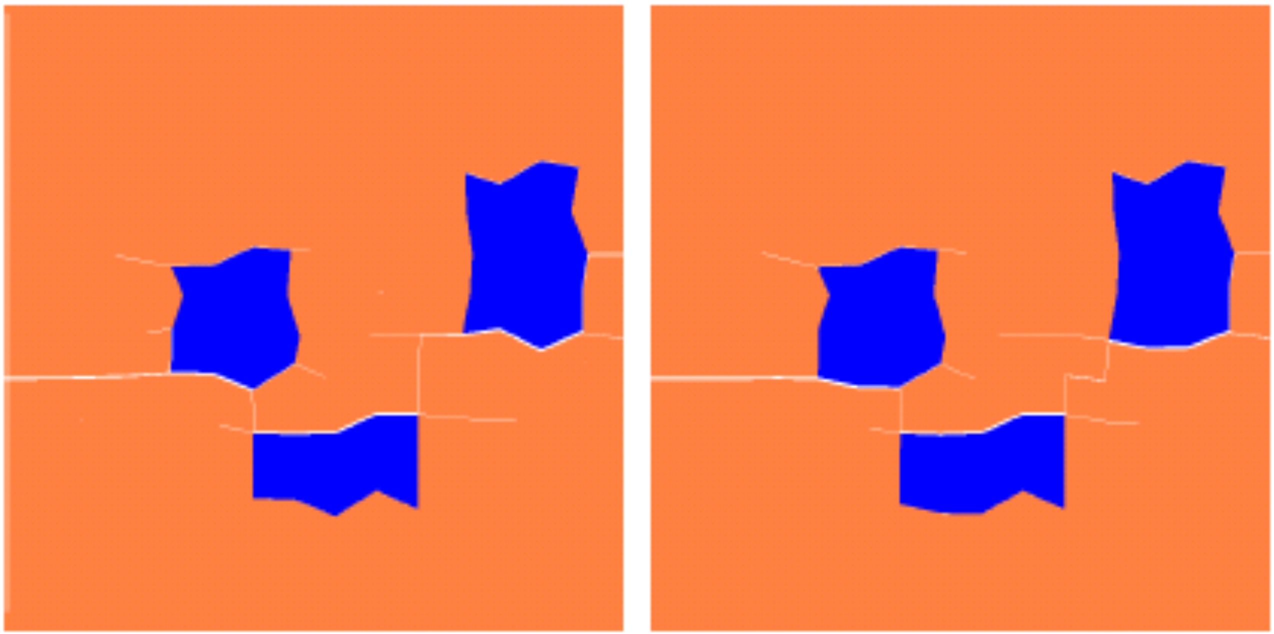
subject to

$$\begin{aligned} -\operatorname{div}\sigma = f \quad &\text{in} \quad \Omega_\gamma, \\ \sigma - A\varepsilon(u) = 0 \quad &\text{in} \quad \Omega_\gamma, \\ u = 0 \quad &\text{on} \quad \Gamma, \end{aligned}$$

$$[u_\nu] \geq 0,\ \sigma_\nu^\pm \leq 0,\ [\sigma_\nu] = 0,\ \sigma_\tau^\pm = 0,\ \sigma_\nu[u_\nu] = 0 \text{ on } \gamma.$$

Problem: this is a two-level optimization problem that may exhibit non-smoothness

BT versus SNOPT

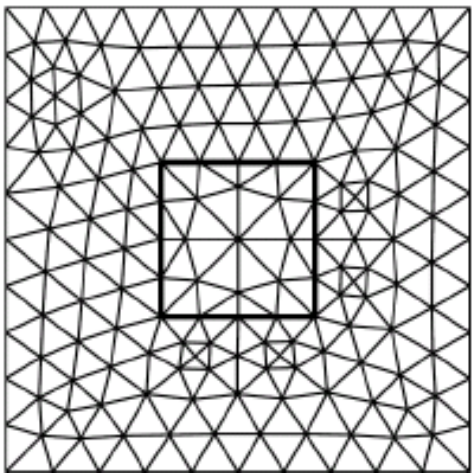


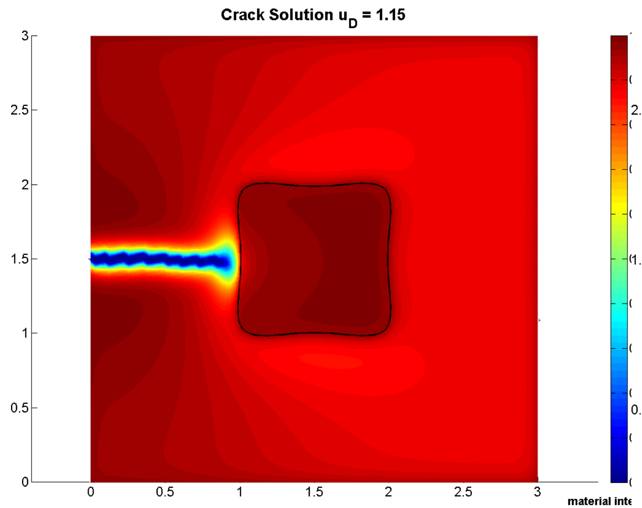
(a) optimal shapes yielded with BT, $W_B = 1.744\text{e-}3$

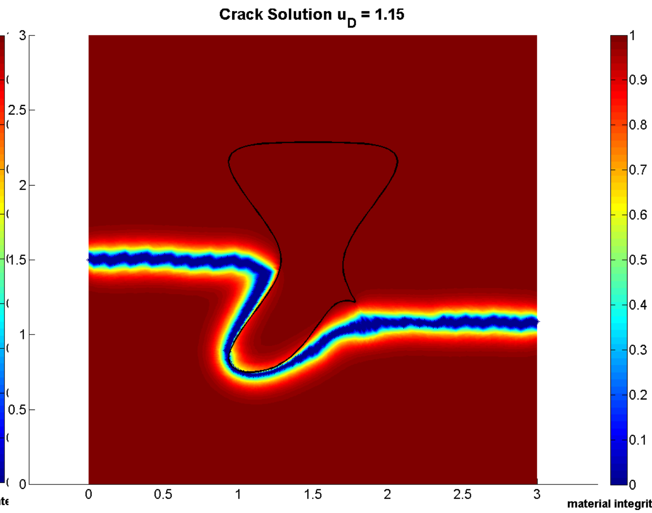
(b) optimal shapes yielded with SNOPT, $W_S = 1.743\text{e-}3$

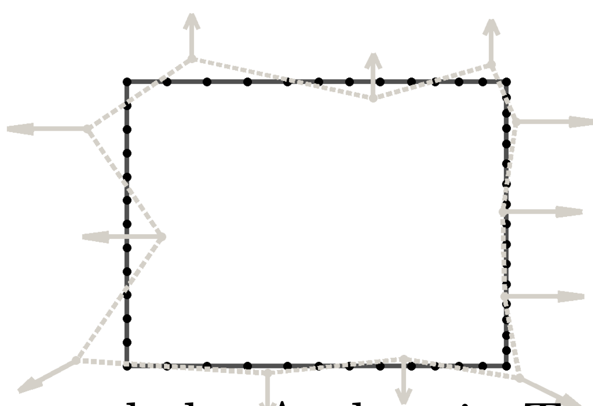
Optimization done with M. Prechtel, P. Steinmann and M. Stingl

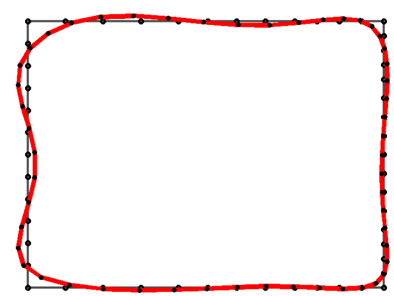
Shape-optimization: parametric





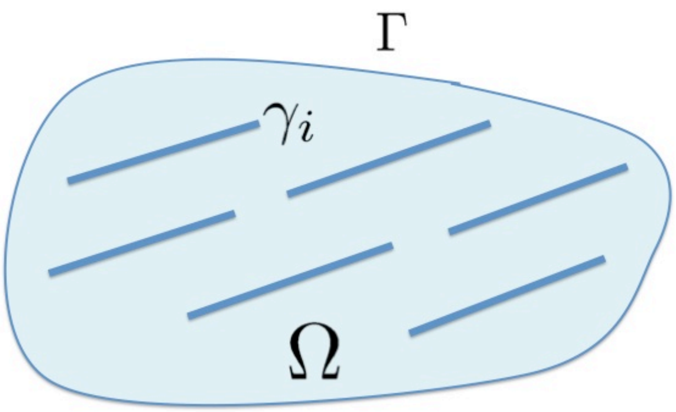






Here we used the Ambrosio-Tortorelli relaxation
Computations by C. Strohmeyer

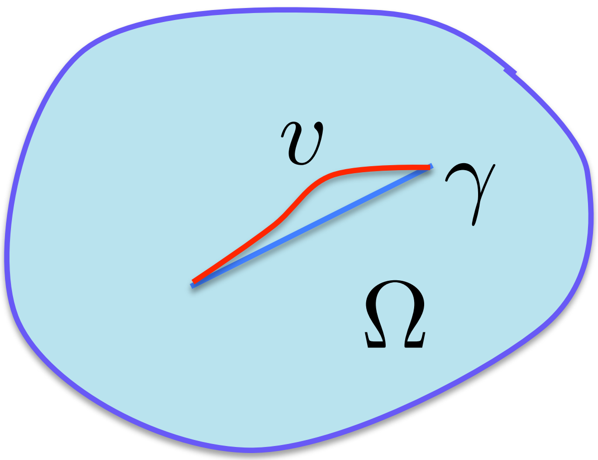
Thin elastic beam inclusion



$$
\begin{aligned}
-\mathrm{div}\, \sigma = f \quad &\text{in} \quad \Omega_\gamma, \\
\sigma - A\varepsilon(u) = 0 \quad &\text{in} \quad \Omega, \\
v_{xxxx} = [\sigma_\nu] \quad &\text{on} \quad \gamma, \\
-w_{xx} = [\sigma_\tau] \quad &\text{on} \quad \gamma, \\
u = 0 \quad &\text{on} \quad \Gamma, \\
v_{xx} = v_{xxx} = w_x = 0 \quad &\text{for} \quad x = 0, 1, \\
v = u_\nu, \; w = u_\tau \quad &\text{on} \quad \gamma.
\end{aligned}
$$

Joint work with A. M. Khludnev 2013

Thin elastic beam inclusion with onsided delamination



$$
\begin{aligned}
-\mathrm{div}\, \sigma = f \quad &\text{in} \quad \Omega_\gamma, \\
\sigma - A\varepsilon(u) = 0 \quad &\text{in} \quad \Omega_\gamma, \\
v_{xxxx} = [\sigma_\nu] \quad &\text{on} \quad \gamma, \\
-w_{xx} = [\sigma_\tau] \quad &\text{on} \quad \gamma, \\
u = 0 \quad &\text{on} \quad \Gamma, \\
v_{xx} = v_{xxx} = w_x = 0 \quad &\text{for} \quad x = 0, 1, \\
[u_\nu] \geq 0,\ v = u_\nu^-,\ w = u_\tau^-,\ \sigma_\nu^+ [u_\nu] = 0 \quad &\text{on} \quad \gamma, \\
\sigma_\nu^+ \leq 0,\ \sigma_\tau^+ = 0 \quad &\text{on} \quad \gamma.
\end{aligned}
$$

Beamstiffness tends to infinity or zero

$\delta \to \infty$

rigid inclusion
with delamination

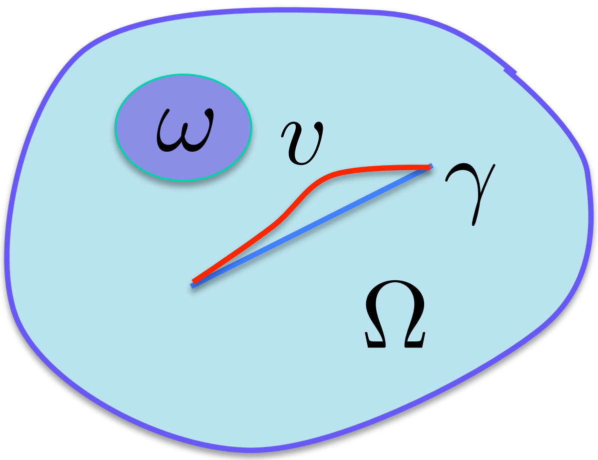
$$
\begin{aligned}
-\mathrm{div}\,\sigma = f \quad & \text{in} \quad \Omega_\gamma, \\
\sigma - A\varepsilon(u) = 0 \quad & \text{in} \quad \Omega_\gamma, \\
u = 0 \quad & \text{on} \quad \Gamma, \\
[u_\nu] \geq 0,\ l_0 = u_\nu^-,\ q_0 = u_\tau^- \quad & \text{on} \quad \gamma, \\
\sigma_\tau^+ = 0,\ \sigma_\nu^+ \leq 0,\ \sigma_\nu^+[u_\nu] = 0 \quad & \text{on} \quad \gamma, \\
\int_\gamma \sigma_\tau^- = 0,\ \int_\gamma [\sigma_\nu] l = 0\ \forall l \in R_s(\gamma).
\end{aligned}
$$

$\delta \to 0$

classical crack

$$
\begin{aligned}
-\mathrm{div}\,\sigma = f \quad & \text{in} \quad \Omega_\gamma, \\
\sigma - A\varepsilon(u) = 0 \quad & \text{in} \quad \Omega_\gamma, \\
u = 0 \quad & \text{on} \quad \Gamma, \\
[u_\nu] \geq 0,\ \sigma_\nu^\pm \leq 0,\ [\sigma_\nu] = 0,\ \sigma_\tau^\pm = 0,\ \sigma_\nu[u_\nu] = 0 \text{ on } \gamma.
\end{aligned}
$$

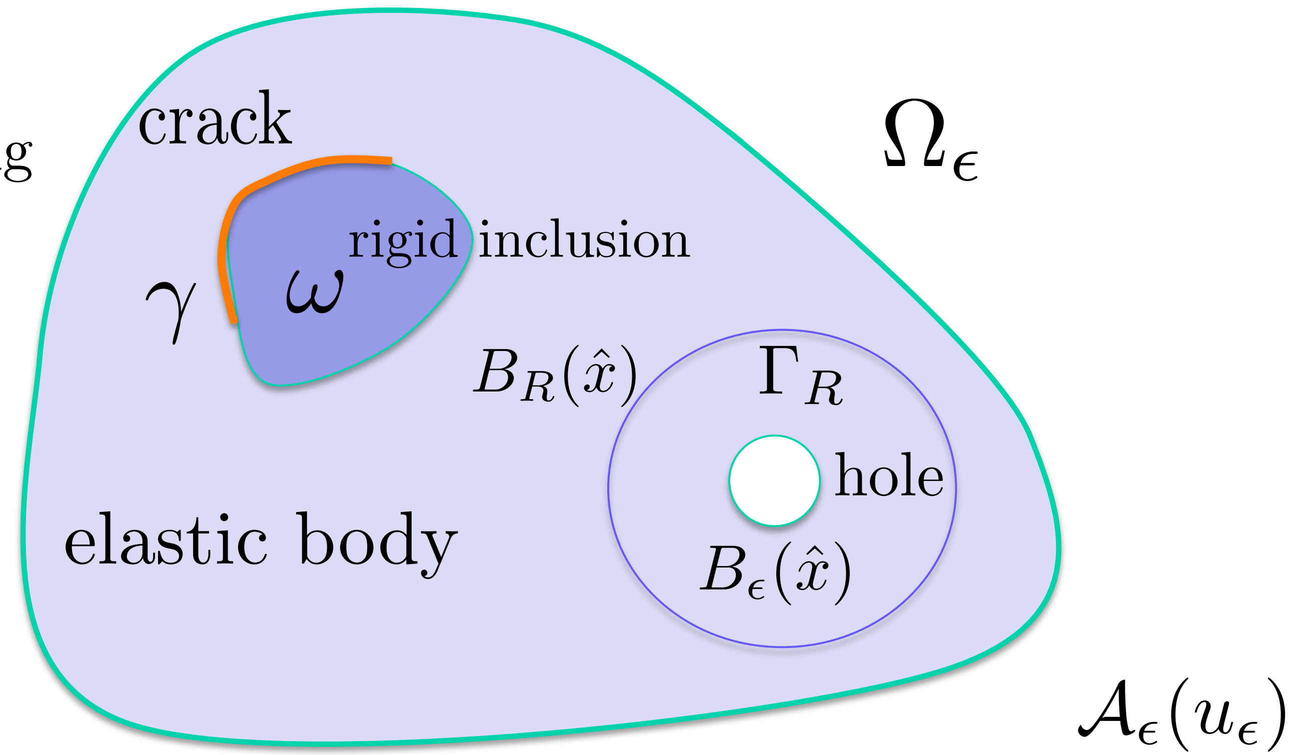
Sensitivity problem



What happens to the delamination when an elastic or rigid inclusion or a hole ω is present?

Crack along rigid inclusion in the presence of a hole
Joint work with Sokolowski and Zochovsky 13'

The influence of the presence of a hole $B_\epsilon(\hat{x})$ on the crack propagation along an interface wit a rigid inclusion ω



compute Steklov-Poincaré operator along Γ_R

Topological sensitivity along inclusion

We are interested in the topological asymptotic expansion of the energy shape functional of the form

$$\mathcal{J}(\Omega_\varepsilon;\varphi) = \frac{1}{2}\int_{\Omega_\varepsilon\setminus\overline{\omega}} \sigma(\varphi)\cdot\nabla\varphi^s - \int_{\Omega_\Upsilon} b\cdot\varphi \ ,$$

with $\varphi = u_\varepsilon$ solution to the following *nonlinear system*

$$\left\{\begin{array}{rcll}
\multicolumn{4}{l}{\text{Find } u_\varepsilon \text{ such that}}\\
-\mathrm{div}\sigma(u_\varepsilon) &=& b & \text{in} \quad \Omega_\varepsilon\setminus\overline{\omega}\ ,\\
\sigma(u_\varepsilon) &=& \mathbb{C}\nabla u_\varepsilon^s\ , & \\
u_\varepsilon &=& 0 & \text{on} \quad \Gamma\ ,\\
\sigma(u_\varepsilon)n &=& 0 & \text{on} \quad \partial B_\varepsilon\ ,\\
\left.\begin{array}{r}(u_\varepsilon-\rho_0)\cdot n \\ \sigma^\tau(u_\varepsilon) \\ \sigma^{nn}(u_\varepsilon) \\ \sigma^{nn}(u_\varepsilon)(u_\varepsilon-\rho_0)\cdot n\end{array}\right. & \begin{array}{c}\geq\\=\\\leq\\=\end{array} & \left.\begin{array}{c}0\\0\\0\\0\end{array}\right\} & \text{on} \quad \Upsilon^+\ ,\\
-\int_{\partial\omega}\sigma(u_\varepsilon)n\cdot\rho &=& \int_\omega b\cdot\rho & \forall \quad \rho\in\mathcal{R}(\omega)\ .
\end{array}\right.$$

The Steklov-Poncaré-operator

We assume that $b = 0$ in $B_R(\widehat{x})$, that is, the source term b vanishes in the neighborhood of the point $\widehat{x} \in \Omega \backslash \overline{\omega}$. Thus, we have the following linear elasticity system defined in the ring $C(R, \varepsilon)$:

$$\left\{ \begin{array}{rcll} \multicolumn{4}{l}{\text{Find } w_\varepsilon \text{ such that}} \\ -\mathrm{div}\sigma(w_\varepsilon) & = & 0 & \text{in} \quad C(R,\varepsilon) \ , \\ \sigma(w_\varepsilon) & = & \mathbb{C}\nabla w_\varepsilon^s \ , & \\ w_\varepsilon & = & v & \text{on} \quad \Gamma_R \ , \\ \sigma(u_\varepsilon)n & = & 0 & \text{on} \quad \partial B_\varepsilon \ , \end{array} \right.$$

where Γ_R is used to denote the exterior boundary ∂B_R of the ring $C(R, \varepsilon)$. We are interested in the Steklov-Poincaré operator on Γ_R, that is

$$\mathcal{A}_\varepsilon : v \in H^{1/2}(\Gamma_R; \mathbb{R}^2) \to \sigma(w_\varepsilon)n \in H^{-1/2}(\Gamma_R; \mathbb{R}^2) \ .$$

The VI with Steklov-Poncare-operator

Then we have $\sigma(u_\varepsilon^R)n = \mathcal{A}_\varepsilon(u_\varepsilon^R)$ on Γ_R, where u_ε^R is solution of the variational inequality in Ω_R, that is

$$u_\varepsilon^R \in \mathcal{K}_\omega : \int_{\Omega_R} \sigma(u_\varepsilon^R) \cdot \nabla(\eta - u_\varepsilon^R) + \int_{\Gamma_R} \mathcal{A}_\varepsilon(u_\varepsilon^R) \cdot (\eta - u_\varepsilon^R) \geq \int_{\Omega_\Upsilon \setminus \overline{B_R}} b \cdot (\eta - u_\varepsilon^R) \quad \forall \eta \in \mathcal{K}_\omega \ .$$

Finally, in the ring $C(R, \varepsilon)$ we have

$$\int_{C(R,\varepsilon)} \sigma(w_\varepsilon) \cdot \nabla w_\varepsilon^s = \int_{\Gamma_R} \mathcal{A}_\varepsilon(w_\varepsilon) \cdot w_\varepsilon \ ,$$

where w_ε is the solution of the elasticity system in the ring. Therefore the solutions u_ε^R and w_ε are defined as restriction of u_ε to the truncated domain Ω_R and to the ring $C(R, \varepsilon)$, respectively.

Expansion of the Steklov-Poincare-op

In the neighborhood of $\widehat{x} \in \Omega \setminus \overline{\omega}$, the energy in the ring $C(R, \varepsilon)$ admits the following topological asymptotic expansion

$$\int_{C(R,\varepsilon)} \sigma(w_\varepsilon) \cdot \nabla w_\varepsilon^s = \int_{B_R} \sigma(w) \cdot \nabla w^s - 2\pi\varepsilon^2 \mathbb{P}\sigma(w(\widehat{x})) \cdot \nabla w^s(\widehat{x}) + o(\varepsilon^2) \; .$$

where w is solution for $\varepsilon = 0$ and $\mathbb{P}$ is the polarization tensor. Therefore, the Steklov-Poincaré operator admits the expansion for $\varepsilon > 0$, with ε small enough,

$$\mathcal{A}_\varepsilon = \mathcal{A} - 2\varepsilon^2 \mathcal{B} + o(\varepsilon^2) \; ,$$

where the operator $\mathcal{B}$ is determined by its bilinear form

$$\langle \mathcal{B}(w), w \rangle_{\Gamma_R} = \pi \mathbb{P}\sigma(w(\widehat{x})) \cdot \nabla w^s(\widehat{x}) \; .$$

Topological derivative

For the energy shape functional associated to the cracks on boundaries of rigid inclusions embedded in elastic bodies we infer

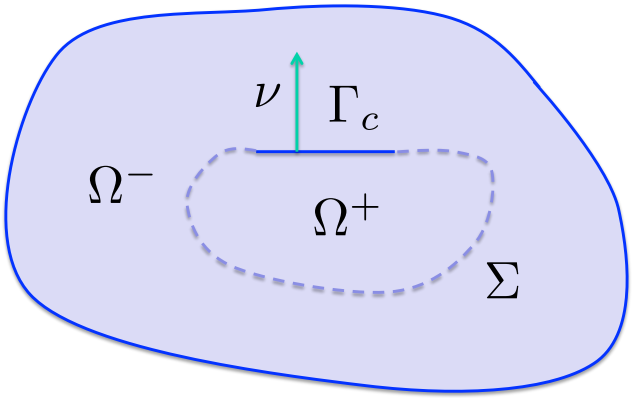
$$\mathcal{J}(\Omega_\varepsilon) = \mathcal{J}(\Omega) - \pi\varepsilon^2 \mathbb{P}\sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) + o(\varepsilon^2) \ ,$$

with the *topological derivative* $\mathcal{T}(\widehat{x})$ given by

$$\mathcal{T}(\widehat{x}) = -\mathbb{P}\sigma(u(\widehat{x})) \cdot \nabla u^s(\widehat{x}) \ ,$$

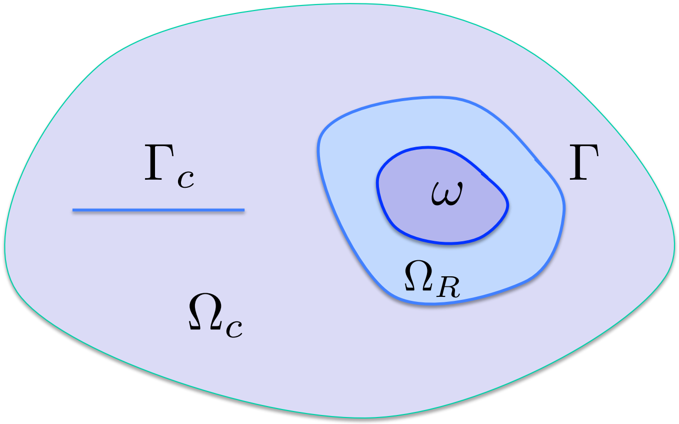
where u is solution of the variational inequality in the unperturbed domain Ω_Υ and $\mathbb{P}$ is the Pólya-Szegö polarization tensor.

DDM for the crack/inclusion problem



DDM for the crack problem:
reduces the to a Signorini-type problem

DDM for the inclusion:
Reduces the crack problem with inclusion zo a problem with nonhomogenous boundary



Shape derivative of potential energy

The energy functional $\mathcal{E}(\Omega_c) = 1/2a(u,u) - (f,u)_{\Omega_c}$ is differentiable in the direction of a vector field V, for the specific choice of the field $V = (v,0)$ the shape derivative

$$V \to d\mathcal{E}(\Omega_c;V) = \frac{1}{t}\lim_{t\to 0}(\mathcal{E}(T_t(\Omega_c)) - (\mathcal{E}(\Omega_c))$$

can be interpreted as the derivative of the elastic energy with respect to the crack length.

Theorem We have

$$d\mathcal{E}(\Omega_c;V) = \frac{1}{2}\int\limits_{\Omega_c} \{\mathrm{div}V \cdot \varepsilon_{ij}(u) - 2E_{ij}(V;u)\}\,\sigma_{ij}(u) - \int\limits_{\Omega_c} \mathrm{div}(V f_i)u_i\,.$$

Shape control of the VI

For a given vector field V supported in a vicinity of the crak Γ_c, denote $2E_{ij}(V;u) := u_{i,k}V_{k,j} + u_{j,k}V_{k,i}$, and define the shape functional depending on ω, with $\Omega = \Omega_\omega \cup \overline{\omega}$,

$$J(\omega) := \frac{1}{2}\int_\Omega \{\mathrm{div}V \cdot \varepsilon_{ij}(u) - 2E_{ij}(V;u)\}\,\sigma_{ij}(u) - \int_\Omega \mathrm{div}(Vf_i)u_i$$

be the shape functional associated with the variational inequality

$$u \in K(\omega), \quad \int_\Omega \sigma_{ij}(u)\varepsilon_{ij}(v-u) \geq \int_\Omega f_i(v_i - u_i), \quad \forall v \in K(\omega),$$

Determine an admissible domain $\omega \subset \Omega_R$ which minimizes $J(\omega)$ over the admissible family.

Steklov-Poincaré

Theorem *Assume that the energy shape functional* $\mathcal{E}(\Omega_R)$ *is shape differentiable in the direction of the velocity field* W *compactly supported in a neighbourhood of the inclusion* $\omega \subset \Omega_R$*, then the Griffith functional is directionally differentiable in the direction of the velocity field* W.

Steklov Poncaré for un-perturbed and perturbed inclusions

$$
\left\{
\begin{array}{rcll}
\multicolumn{4}{l}{\text{Find } u, \text{ such that}} \\
\mathrm{div}\sigma(u) & = & 0 & \text{in} \quad \Omega \,, \\
\sigma(u) & = & \mathbb{C}\nabla u^s \,, & \\
u & = & \overline{u} & \text{on} \quad \Gamma_D \,, \\
\sigma(u)n & = & \overline{q} & \text{on} \quad \Gamma_N \,.
\end{array}
\right.
$$

$$
\left\{
\begin{array}{rcll}
\multicolumn{4}{l}{\text{Find } u_\varepsilon, \text{ such that}} \\
\mathrm{div}\sigma_\varepsilon(u_\varepsilon) & = & 0 & \text{in} \quad \Omega \,, \\
\sigma_\varepsilon(u_\varepsilon) & = & \gamma_\varepsilon \mathbb{C}\nabla u^s_\varepsilon \,, & \\
u_\varepsilon & = & \overline{u} & \text{on} \quad \Gamma \,, \\
u_\varepsilon & = & 0 & \text{on} \quad \Gamma_D \,, \\
\sigma(u_\varepsilon)n & = & 0 & \text{on} \quad \Gamma_N \,, \\
[\![u_\varepsilon]\!] & = & 0 & \\
[\![\sigma_\varepsilon(u_\varepsilon)]\!] n & = & 0 & \Big\} \ \text{on} \quad \partial B_\varepsilon \,.
\end{array}
\right.
$$

Shape functional

Let us introduce the, namely

$$\mathbb{E}_\varepsilon = \frac{1}{2}(\sigma_\varepsilon(u_\varepsilon) \cdot \nabla u_\varepsilon^s)\mathrm{I} - \nabla u_\varepsilon^\top \sigma_\varepsilon(u_\varepsilon) \ .$$

In addition, we note that after considering the constitutive relation $\sigma_\varepsilon(u_\varepsilon) = \gamma_\varepsilon \mathbb{C} \nabla u_\varepsilon^s$ with the contrast γ_ε, the shape functional $\psi(\chi_\varepsilon)$ can be written as follows

$$\psi(\chi_\varepsilon) = \frac{1}{2}\left(\int_{\Omega \setminus \overline{B_\varepsilon}} \sigma(u_\varepsilon) \cdot \nabla u_\varepsilon^s + \int_{B_\varepsilon} \gamma \sigma(u_\varepsilon) \cdot \nabla u_\varepsilon^s\right) ,$$

where $\sigma(u_\varepsilon) = \mathbb{C} \nabla u_\varepsilon^s$. Therefore, the explicit dependence with respect to the parameter ε arises.

Shape derivative in a special case

The shape derivative of $\psi(\chi_\varepsilon)$ with respect to the small parameter ε is given by

$$\dot{\psi}(\chi_\varepsilon) = \int_{\partial B_\varepsilon} [\![\mathbb{E}_\varepsilon]\!] n \cdot \mathfrak{V} \, , \tag{1}$$

with $\mathfrak{V}$ standing for the shape change velocity field compactly supported in a neighbourhood of ∂B_ε and tensor $\mathbb{E}_\varepsilon$