Method-of-Moments-Based Memetics for Inverse Design

Miloslav Čapek[1], Lukáš Jelínek[1], Vojtěch Neuman[1], Jonáš Tuček[1], Petr Kadlec[2], and Mats Gustafsson[3]

[1]Department of Electromagnetic Field
Czech Technical University in Prague
Czech Republic
miloslav.capek@fel.cvut.cz

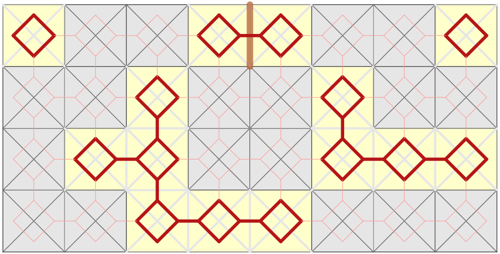
[2]Department of Radio Electronics
Brno University of Technology
Czech Republic

[3]Department of Electrical and Information Technology
Lund University
Sweden

November 23, 2021
Workshop on Modern Optimization and Machine Learning II
Lund

Outline

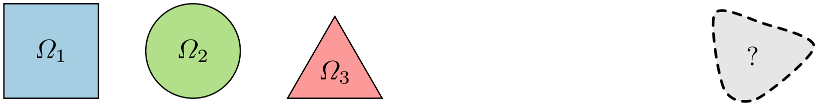
1. Topology Optimization
2. Memetic Scheme
3. Examples
4. Regularity – Geometrical Operators in MoM
5. Conclusion



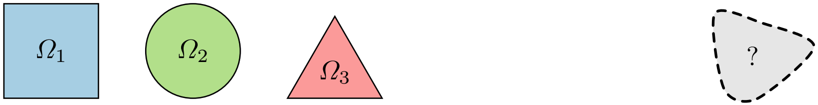
$i = 0,\ Q/Q_{\mathrm{lb}}^{\mathrm{TM}} = 119.35$

Download the presentation from: capek.elmag.org.

Topology Optimization as Inverse Design Problem



Topology Optimization as Inverse Design Problem



- shape optimization × topology optimization
- NP hard problem (unsolvable in its entirety)
- synthesis of beam-steering arrays, optimal antennas, metasurfaces, and more...

Contemporary Approaches

Local methods (*e.g.*, adjoint method)

- deterministic
- fast convergence
- does always "the best" move

Global methods, (*e.g.*, heuristics)

- robust
- prevent stacking in local minima
- maintain diversity

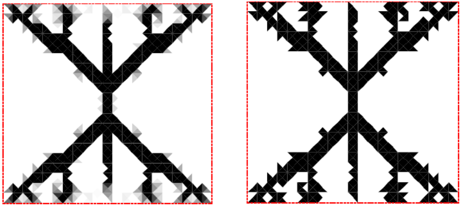
Contemporary Approaches

Local methods (*e.g.*, adjoint method)

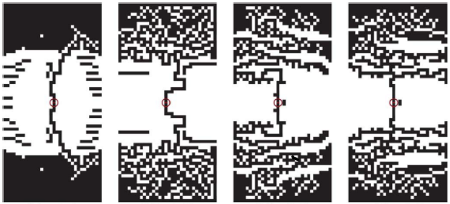
- deterministic
- fast convergence
- does always "the best" move

Global methods, (*e.g.*, heuristics)

- robust
- prevent stacking in local minima
- maintain diversity



Topology optimization of a bowtie[1].



Antenna design with genetic algorithm[2].

[1] S. Liu, Q. Wang, and R. Gao, "MoM-based topology optimization method for planar metallic antenna design," *Acta Mechanica Sinica*, vol. 32, no. 6, pp. 1058–1064, 2016. DOI: 10.1007/s10409-016-0584-0

[2] M. Cismasu and M. Gustafsson, "Antenna bandwidth optimization with single frequency simulation," *IEEE Trans. Antennas Propag.*, vol. 62, no. 3, pp. 1304–1311, 2014

Memetic Approach – Future of Antenna Design?

Evaluating all local perturbations of the MoM model...

- Local step: fast detection of local minima.
- Global step: operates in local minima subspace only.

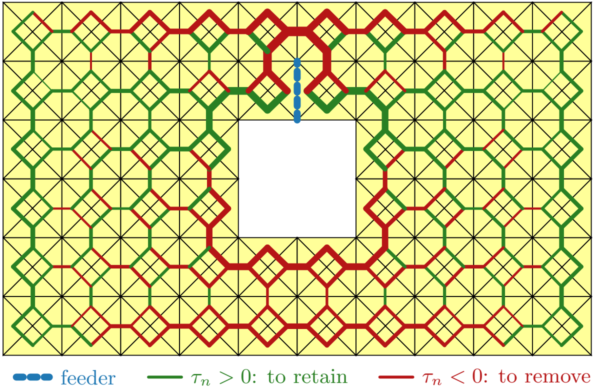
Memetic Approach – Future of Antenna Design?

Evaluating all local perturbations of the MoM model...

- Local step: fast detection of local minima.
- Global step: operates in local minima subspace only.

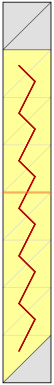
Properties:

- fast, versatile, and full-wave,
- removes disadvantages of the existing methods,
- generates big data,
- combination of metrics, multi-frequency, multi-port.



Topology sensitivities as seen during the optimization.

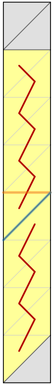
Novel Local Approach Based on Exact Re-analysis



$$\begin{bmatrix} Z_{11} & Z_{12} & \cdots & Z_{1M} & \cdots & Z_{1N} \\ Z_{21} & Z_{22} & \cdots & Z_{2M} & \cdots & Z_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ Z_{M1} & Z_{M2} & \cdots & \infty & \cdots & Z_{MN} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ Z_{N1} & Z_{N2} & \cdots & Z_{NM} & \cdots & Z_{NN} \end{bmatrix}$$

$$\mathbf{Y} = \mathbf{Z}^{-1}$$

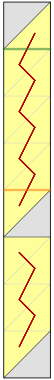
$$\begin{bmatrix} Y_{11} & Y_{12} & \cdots & 0 & \cdots & Y_{1N} \\ Y_{21} & Y_{22} & \cdots & 0 & \cdots & Y_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ Y_{N1} & Y_{N2} & \cdots & 0 & \cdots & Y_{NN} \end{bmatrix}$$



$$\begin{bmatrix} \infty & Z_{12} & \cdots & Z_{1M} & \cdots & Z_{1N} \\ Z_{21} & Z_{22} & \cdots & Z_{2M} & \cdots & Z_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ Z_{M1} & Z_{M2} & \cdots & \infty & \cdots & Z_{MN} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ Z_{N1} & Z_{N2} & \cdots & Z_{NM} & \cdots & Z_{NN} \end{bmatrix}$$

$$\hat{\mathbf{Y}} = \hat{\mathbf{Z}}^{-1} = \mathbf{Y} - \frac{1}{Y_{11}} \mathbf{y}_1 \mathbf{y}_1^{\mathrm{T}}$$

$$\begin{bmatrix} 0 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & Y_{22} & \cdots & 0 & \cdots & Y_{2N} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & Y_{N2} & \cdots & 0 & \cdots & Y_{NN} \end{bmatrix}$$



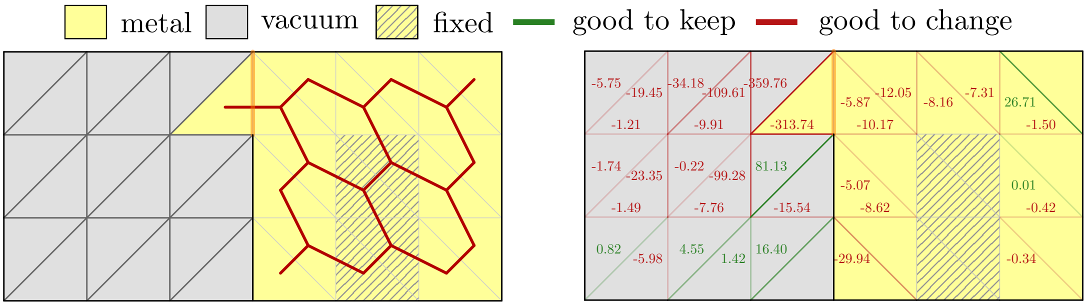
$$\begin{bmatrix} \infty & Z_{12} & Z_{13} & \cdots & Z_{1N} & Z_{1M} \\ Z_{21} & \infty & Z_{23} & \cdots & Z_{2N} & Z_{2M} \\ Z_{31} & Z_{32} & Z_{33} & \cdots & Z_{3N} & Z_{3M} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ Z_{N1} & Z_{N2} & Z_{N3} & \cdots & Z_{NN} & Z_{NM} \\ Z_{M1} & Z_{M2} & Z_{M3} & \cdots & Z_{MN} & Z_{MM} \end{bmatrix}$$

$$\hat{\mathbf{Y}} = \hat{\mathbf{Z}}^{-1} = \frac{1}{z_M} \begin{bmatrix} z_M \mathbf{Y} + \mathbf{x}_M \mathbf{x}_M^{\mathrm{T}} & -\mathbf{x}_M \\ -\mathbf{x}_M & 1 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & Y_{33} & \cdots & Y_{3N} & Y_{3M} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & Y_{N3} & \cdots & Y_{NN} & Y_{NM} \\ 0 & 0 & Y_{M3} & \cdots & Y_{7M} & Y_{MM} \end{bmatrix}$$

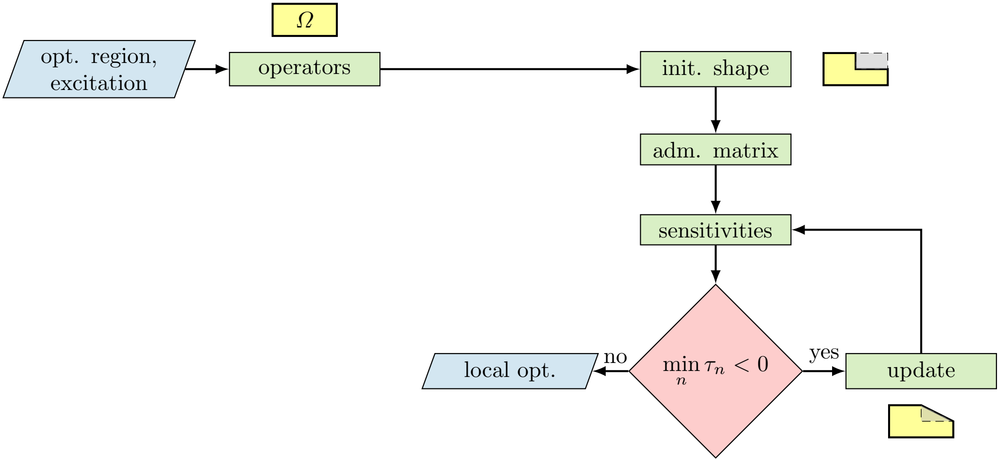
- All possible removals/additions calculated fast, no inversion needed.

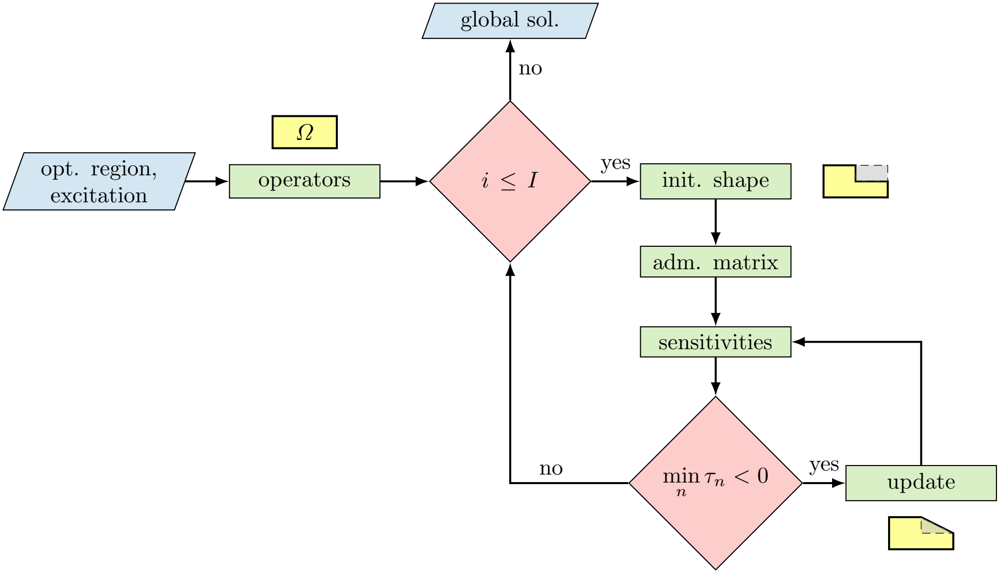
Local, Inversion-Free, and Gradient-Based Update

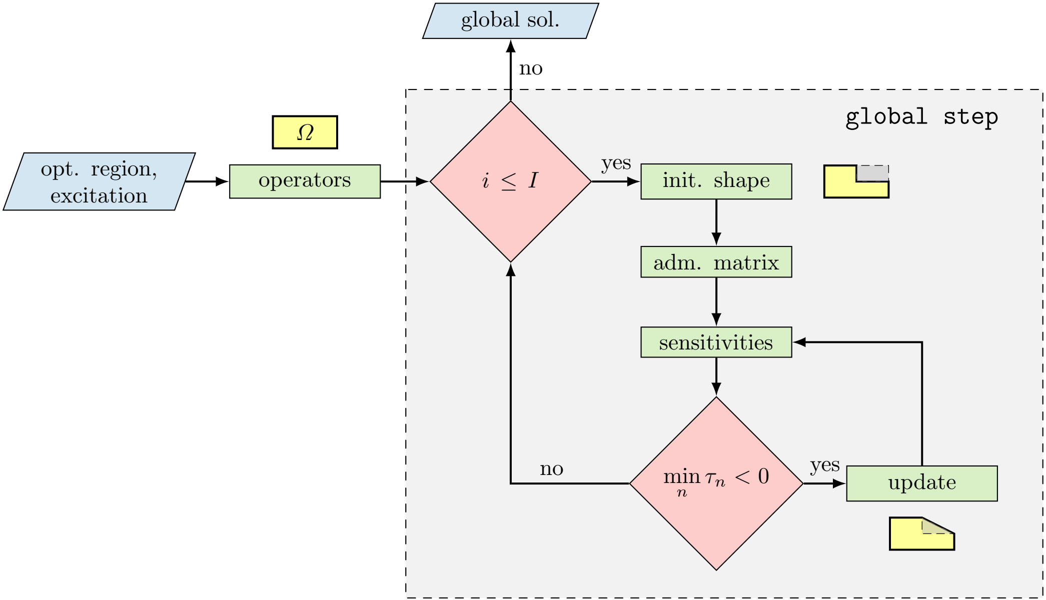


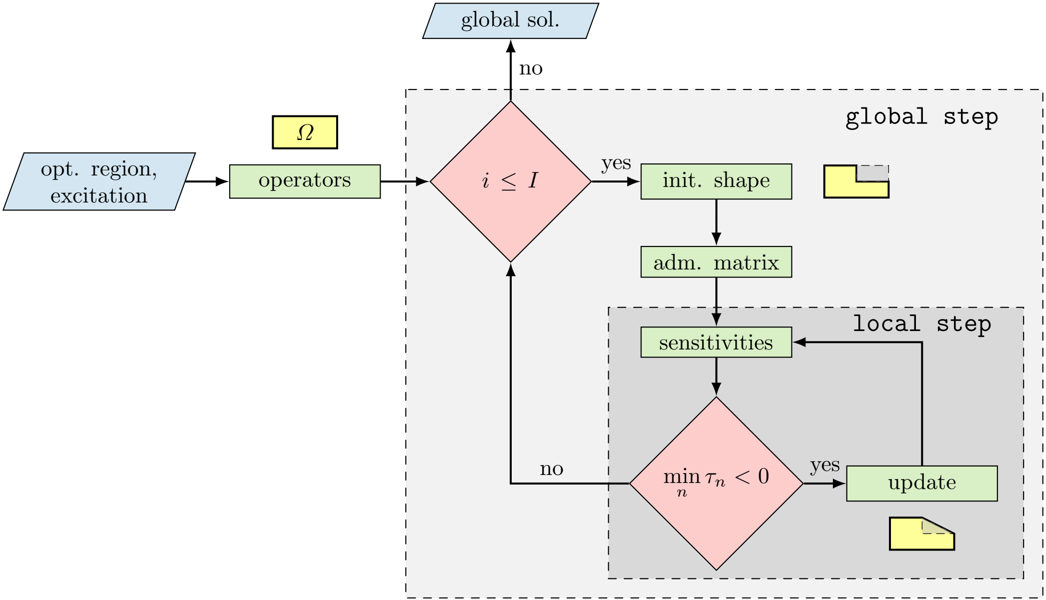
$i = 0$

- The worst element always updated.
- No gray elements (like in adjoint formulation).
- Combinatorial problem solved in a local sense.


Ω
opt. region, excitation
operators
init. shape
adm. matrix
sensitivities
min_n τ_n < 0
no
yes
local opt.
update


global sol.
no
Ω
opt. region,
excitation
operators
$i \leq I$
yes
init. shape
adm. matrix
sensitivities
no
$\min_n \tau_n < 0$
yes
update


global sol.
no
global step
Ω
opt. region, excitation
operators
$i \leq I$
yes
init. shape
adm. matrix
sensitivities
$\min_n \tau_n < 0$
no
yes
update


global sol.
no
global step
Ω
opt. region, excitation
operators
$i \leq I$
yes
init. shape
adm. matrix
local step
sensitivities
no
$\min_n \tau_n < 0$
yes
update

For further details. . .

Memetic Scheme for Inverse Design Using Exact Reanalysis of Method-of-Moments Models – Part 1: Theory and Implementation

Miloslav Capek, *Senior Member, IEEE*, Lukas Jelinek, Petr Kadlec, and Mats Gustafsson, *Senior Member, IEEE*

***Abstract*—A novel inverse design framework over a fixed discretization grid using method of moments for the shape optimization of radiation devices is proposed. The formulation is discrete and solves the original combinatorial problem. Fixed discretization provides an inversion-free, exact-reanalysis-based evaluation of the smallest topology perturbations. The fixed grid also allows to precalculate all expensive evaluations prior to the optimization. Local greedy-based structural updates are combined with global, heuristic steps, resulting in a rapidly converging and robust memetic algorithm applicable to various problems of electromagnetic inverse design. The method is robust and versatile, capable of evaluating a vast amount of possible shapes in a full-wave manner. It shows superb performance over widely used heuristic approaches, such as genetic algorithms or swarm optimization. Thanks to the discrete formulation, no filtering or rounding is needed as compared to the adjoint formulation of topology optimization.**

***Index Terms*—Antennas, numerical methods, optimization methods, shape sensitivity analysis, structural topology design, inverse design.**

I. Introduction

SHAPE optimization is a long-lasting subject of study in electromagnetism. This is particularly true for antenna design [1], the art of crafting and shaping the material to modify electric current paths and dislocate the electromagnetic (EM) sources so that they radiate effectively.

Various procedures [2] have been proposed and met with mixed success, ranging from simple parametric sweeps to versatile heuristic algorithms [3] to powerful topology optimization [4]. All these methods embody serious practical weaknesses, mainly due to the NP-hard problems faced [5]

The specific formulation of shape optimization also strongly depends on a numerical method utilized to quantify the EM interaction [7]. For example, topology optimization stemming from mechanical engineering is best prepared for the finite element method (FEM) [8], although some attempts to transpose its advantages into the finite-difference time-domain method (FDTD) [9] or method of moments (MoM) paradigm [10] are reported. The same is true for sensitivity analysis and gradient-based local optimization [11], [9] which benefit from FEM formulation.

Another example is pixeling techniques [12], typically powered by genetic algorithms [12] which most commonly uses MoM impedance matrices [13], coding each discretization element (simplex "pixels") as one binary unknown that is enabled (the pixel is made from a given material) or disabled (the pixel is made from the vacuum). The link to MoM becomes even more pronounced when discretization elements and EM unknowns are the optimization variables, *i.e.*, the degrees-of-freedom (DOF) for solving the EM problems are identical to those used for optimization. Then, the solver MoM can be inserted inside the optimizer, making it possible to accelerate the solution of the EM problem during the optimization [14].

Apart from the methods discussed above, a broad class of design paradigms utilizes parametric sweeps, surrogate models [15], [16], or design libraries [17]. These tools are efficient as long as a device's shape is predetermined by a set of parameters, *i.e.*, a designer has a clear idea of its topology. Then, the task is to optimize a set of continuous design parameters for which modern tools, such as machine

Memetic Scheme for Inverse Design Using an Exact Reanalysis of Method-of-Moments Models – Part 2: Examples and Properties

Miloslav Capek, *Senior Member, IEEE*, Lukas Jelinek, Petr Kadlec, and Mats Gustafsson, *Senior Member, IEEE*

***Abstract*—Memetics for shape synthesis, introduced in the Part 1, is examined on antenna design examples. It combines local and global techniques to accelerate convergence and to maintain robustness. Method-of-moments matrices are used to evaluate objective functions. By applying the Shermann-Morrison-Woodbury identity, the repetitively performed structural update is inversion-free yet full-wave in nature. The technique can easily be combined with additional features often required in practice, *e.g.*, only a part of the structure is controllable or evaluation of an objective function is required in a subdomain only. The framework supports multi-frequency and multi-port optimization, and offers many other advantages, such as an actual shape being known at every moment of the optimization. The performance of the method is assessed, including its convergence and computational cost.**

***Index Terms*—Antennas, numerical methods, optimization methods, shape sensitivity analysis, structural topology design, inverse design.**

I. Introduction

INVERSE design (shape optimization) is a time-consuming process with no certainty regarding global minimum feasibility [1]. This is always the case, no matter how sophisticated the method employed [2], [3], [4], [5], [6], [7], [8], [9]. There is no theoretical proof of convergence of the shape optimization problem towards the global minimum [2], [3]. However, the global minimum is typically not needed in practice. A sufficiently good solution has to be found in a reasonable time. As such, a good balance between detailed local search and large-scale exploration of the solution space has to be achieved [10]. These properties are provided by the approach introduced in Part 1 [11] which lays down the

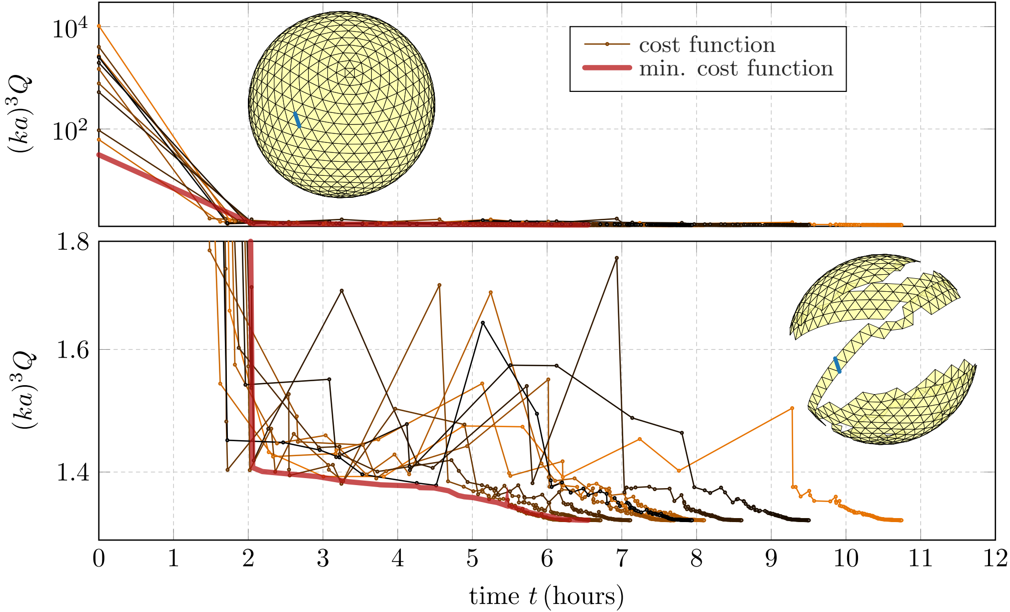
local step was proposed in [12], where only DOF removals were used to detect the local minima. The approach was extended by the possibility of adding DOF to the system in [13]. Satisfactory performance of the local step was confirmed on Q-factor minimization [13], as well as on the minimization of reflectance of a pixel antenna [14]. Part 1 [11] merged both smallest perturbations (addition and removal of DOF) into a unified framework and combined it with the global step.

Since a fixed discretization grid is used, the differences calculated from the change of the objective function value under the smallest topology perturbations (topology sensitivites) represent a discrete analogue to gradient over structural variables. As with gradient-based convex optimization schemes, these differences are used to search for a local minimum via an iterative greedy search [15].

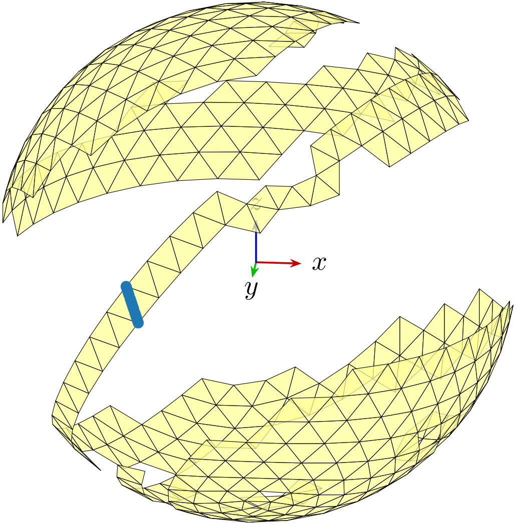
The global step is designed to restore and maintain diversity when the local minima are found by the local step. Therefore, a heuristics known for its robustness is adopted [16], [17] in the form of a genetic algorithm operating over locally optimal shapes. The binary nature of genetics suits the combinatorial-type optimization solved in this work. While heuristics do not, in general, perform well [18], only good properties, including versatility, robustness and easy implementation, are used here while the disadvantages (mainly computational requirements and slow convergence [19]) are mitigated by the underlying local step. Moreover, it is shown in this paper that, in many cases, only the local step is needed to identify shapes good enough for practical purposes. The above-mentioned properties and claims are confirmed in this paper using four examples involving electrically small and medium-size problems. Both

Part 1, https://arxiv.org/abs/2110.08044 Part 2, https://arxiv.org/abs/2110.13460

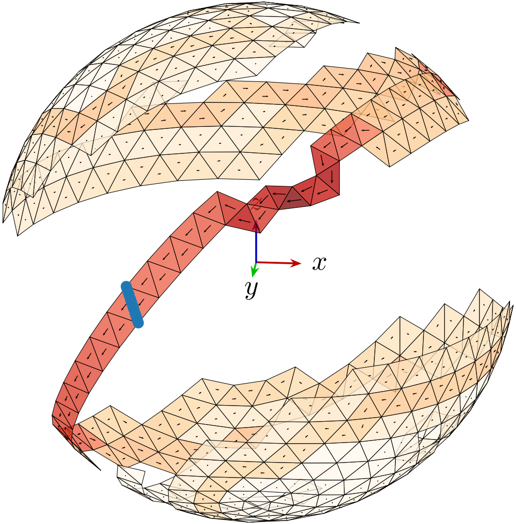
Example #1: Maximal Bandwidth (RWG surface code)



Example #1: Maximal Bandwidth (Optimal Structures)

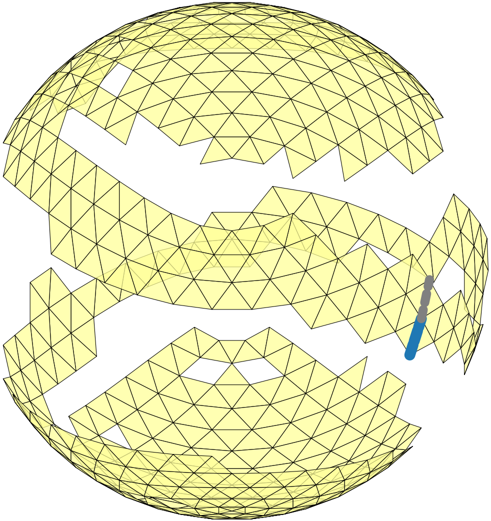


Optimal structure ($N = 2304$, $ka = 0.2$).

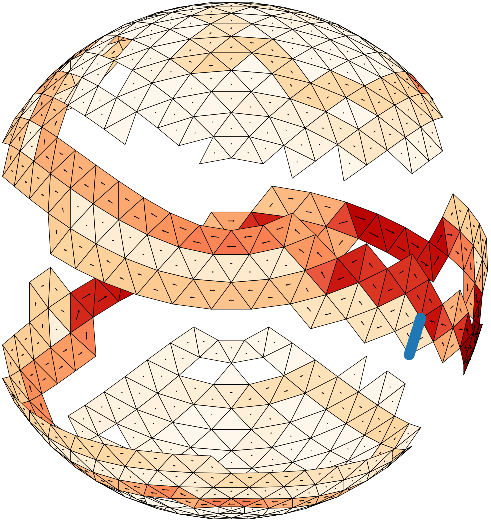


Optimal current ($Q/Q_{\mathrm{lb}} = \mathbf{1.27}$, $Z_{\mathrm{in}} = 2.14\,\Omega$).

Example #1: Maximal Bandwidth & Good Matching

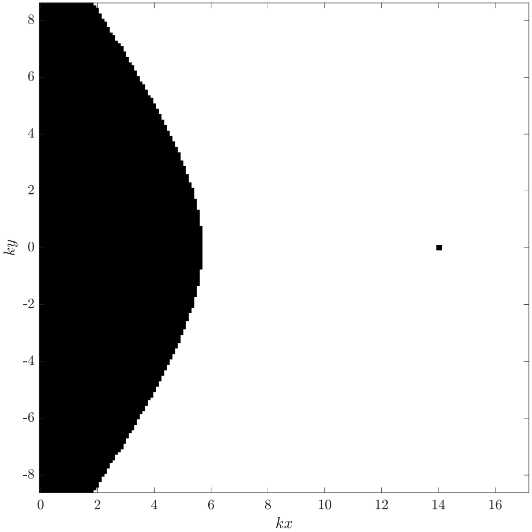


Optimal structure ($N = 2304$, $ka = 0.2$).



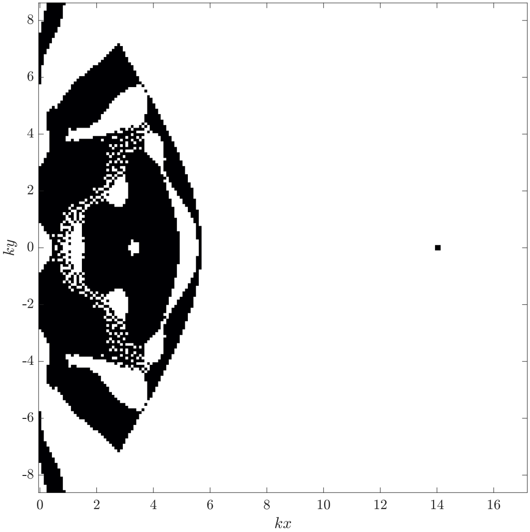
Optimal current ($Q/Q_{\mathrm{lb}} = 1.27$, $Z_{\mathrm{in}} = \mathbf{51.5 - 2.39}\mathrm{j}\,\Omega$).

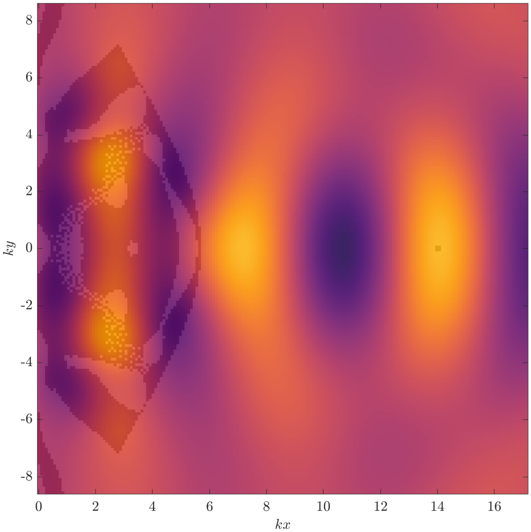
Example #2: Lensing Problem (2D code, transversal E_z field)



$\varepsilon_\mathrm{r} = 3 - 0.06\mathrm{j}$, $N = 8000$, $t \approx 1\,\mathrm{hour}$, sym. used.

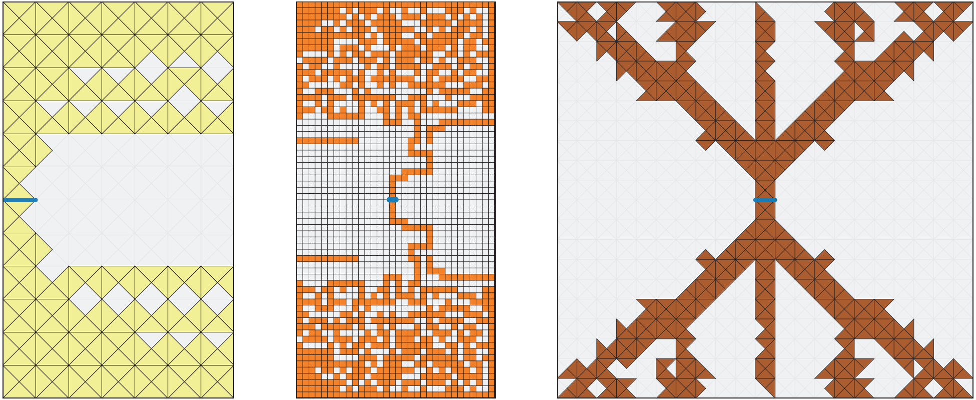
Example #2: Lensing Problem (2D code, transversal E_z field)





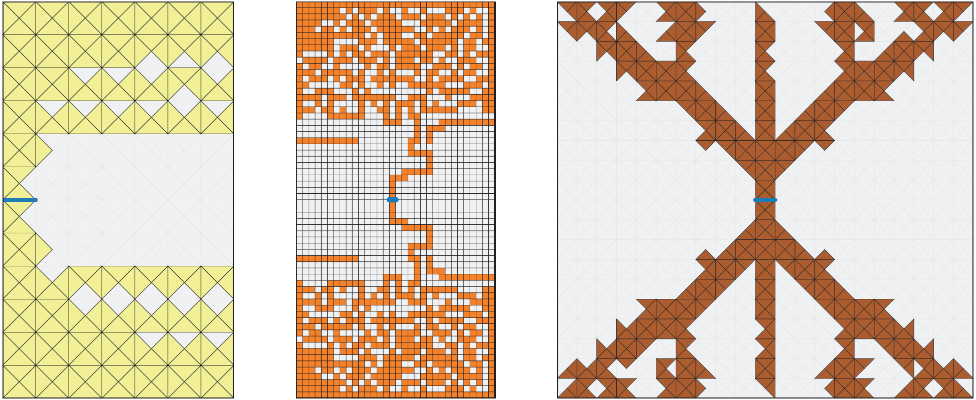
$P_{\mathrm{orig}}/P_{\mathrm{ub}} = \mathbf{0.66}$ vs. $P_{\mathrm{optim}}/P_{\mathrm{ub}} = \mathbf{0.80}$.

Regularity



Left to right: this talk (memetics), genetic algorithms (pixeling), topology optimization (adjoint formulation).

Regularity

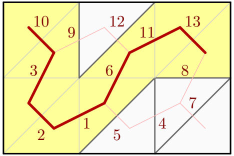


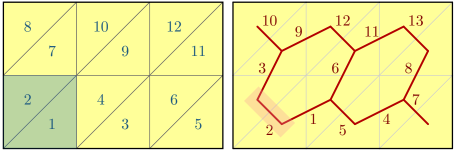
Left to right: this talk (memetics), genetic algorithms (pixeling), topology optimization (adjoint formulation).

- What is regular? How to measure regularity?

Shape Representation and Graph Theory

1. A map between material elements (discretization) and degrees of freedom (basis functions).



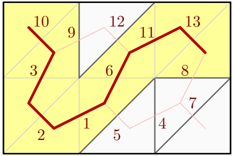


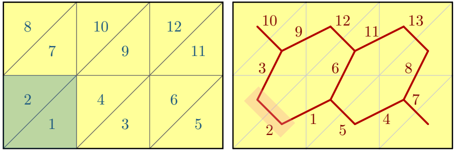
$$\boldsymbol{t}_i = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \end{bmatrix}^{\mathrm{T}}$$

$$\boldsymbol{g}_i = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \end{bmatrix}^{\mathrm{T}}$$

Shape Representation and Graph Theory

1. A map between material elements (discretization) and degrees of freedom (basis functions).
2. Incidence matrix **M** (graph theory).



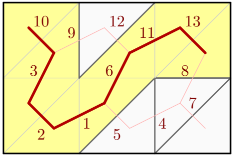


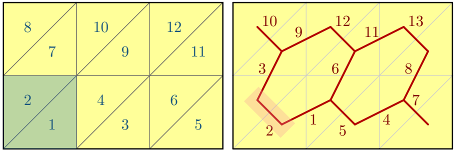
$$\boldsymbol{t}_i = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \end{bmatrix}^{\mathrm{T}}$$
$$\boldsymbol{g}_i = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \end{bmatrix}^{\mathrm{T}}$$

Shape Representation and Graph Theory

1. A map between material elements (discretization) and degrees of freedom (basis functions).
2. Incidence matrix **M** (graph theory).

$$\mathbf{M} = \begin{bmatrix} 1 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 1 & 1 & & 0 \\ 0 & 0 & 0 & 0 & & 0 \\ \vdots & & & & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$





$$\boldsymbol{t}_i = \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \end{bmatrix}^{\mathrm{T}}$$

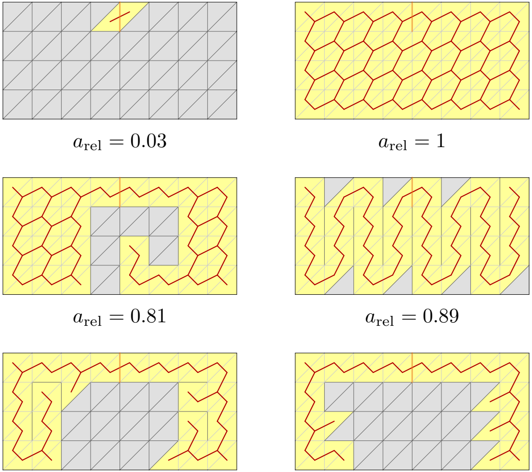
$$\boldsymbol{g}_i = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 \end{bmatrix}^{\mathrm{T}}$$

Relative Area Spanned by a Device

We usually want as small device as possible.

- Area spanned by the metalization:

$$A(\boldsymbol{g}_i) = \mathbf{a}^{\mathrm{T}} \boldsymbol{t}_i = \mathbf{a}^{\mathrm{T}} \mathcal{B}(\mathbf{M}\boldsymbol{g}_i).$$



$a_{\mathrm{rel}} = 0.03$ $a_{\mathrm{rel}} = 1$

$a_{\mathrm{rel}} = 0.81$ $a_{\mathrm{rel}} = 0.89$

$a_{\mathrm{rel}} = 0.66$ $a_{\mathrm{rel}} = 0.53$

$\mathbf{a}$: vector of element areas/volumes
$\mathcal{B}(\cdot)$: Boolean operator (nonzeros $\to$ 1, 0 $\to$ 0)

Shape Regularity

We usually want as regular shape as possible.

- Regularity of the shape

$$r_{\mathrm{reg}}(\boldsymbol{g}_i) = 1 - \frac{1}{N} \left\| \boldsymbol{g}_0 - 2\widetilde{\mathbf{H}}\boldsymbol{g}_i \right\|_1 ,$$

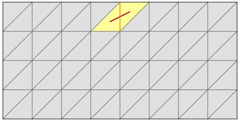
where adjacency matrix is

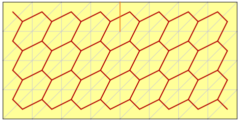
$$\mathbf{H} = \mathcal{B}(\mathbf{M}^{\mathrm{T}}\mathbf{M})$$

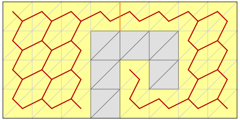
and

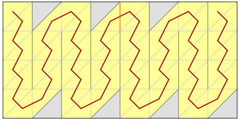
$$\widetilde{\mathbf{H}} = \left[\frac{\mathbf{h}_1}{\|\mathbf{h}_1\|_1} \quad \cdots \quad \frac{\mathbf{h}_j}{\|\mathbf{h}_j\|_1} \quad \cdots \quad \frac{\mathbf{h}_N}{\|\mathbf{h}_N\|_1} \right]^{\mathrm{T}} .$$

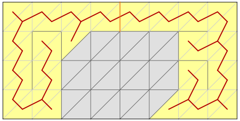
N: number of DOFs

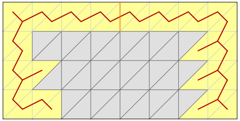

$r_{\mathrm{reg}} = 0.02$


$r_{\mathrm{reg}} = 0$


$r_{\mathrm{reg}} = 0.23$


$r_{\mathrm{reg}} = 0.66$

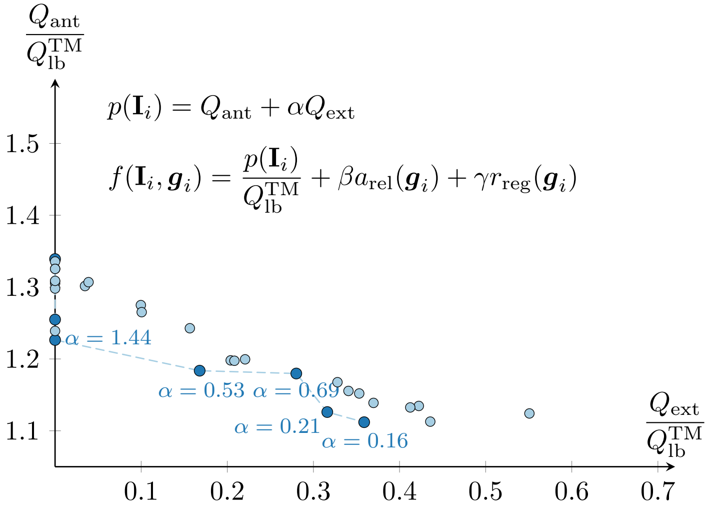

$r_{\mathrm{reg}} = 0.3$


$r_{\mathrm{reg}} = 0.25$

Performance × Appearance Trade-off

Bandwidth Maximization vs. Tuning

- $7 \cdot 10^4$ shapes/s (PC)
- $8 \cdot 10^5$ shapes/s (cluster)

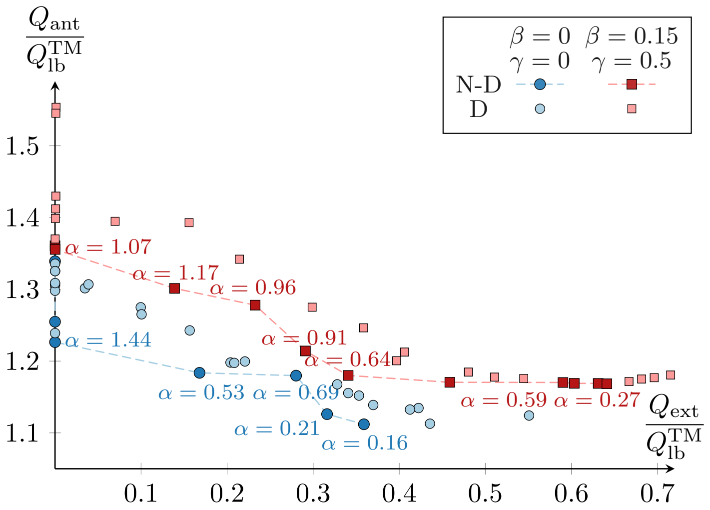


- $ka = 1/2$, PEC, $N = 414$

Performance × Appearance Trade-off

Bandwidth Maximization vs. Tuning

- $7 \cdot 10^4$ shapes/s (PC)
- $8 \cdot 10^5$ shapes/s (cluster)

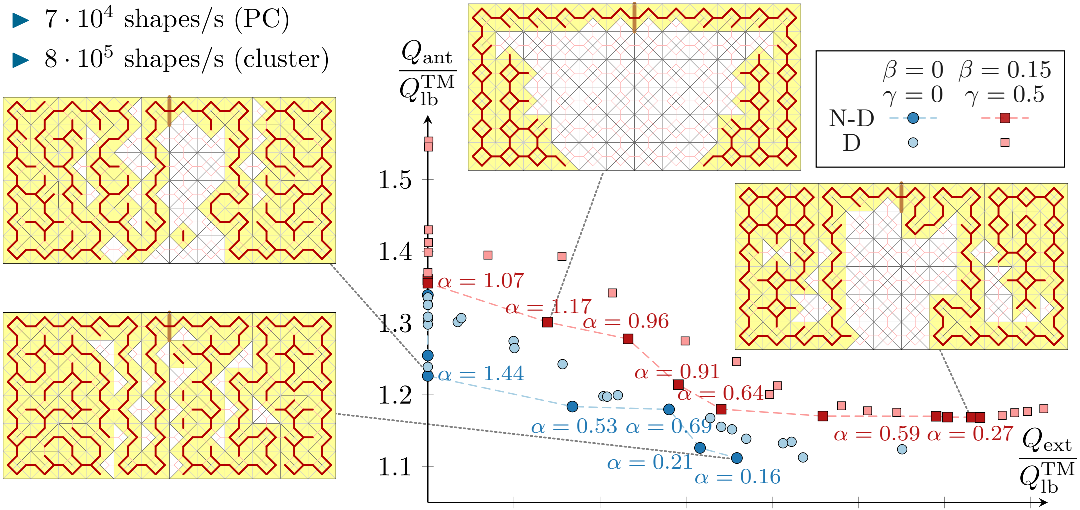


- $ka = 1/2$, PEC, $N = 414$

Performance × Appearance Trade-off

Bandwidth Maximization vs. Tuning

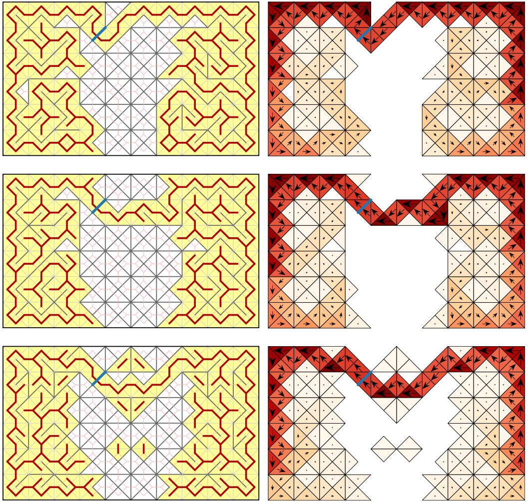
- $7 \cdot 10^4$ shapes/s (PC)
- $8 \cdot 10^5$ shapes/s (cluster)



- $ka = 1/2$, PEC, $N = 414$

Penalization for Asymmetry

Reflection along y-z plane.



From top to bottom: $w = 0$, $w = 0.03$, $w = 1$.

Point group symmetry operation R is

$$R\psi_m(\boldsymbol{r}) = \sum_{n=1}^{N} C_{mn}(R)\,\psi_n(\boldsymbol{r}).$$

Symmetricity $r_{\mathrm{sym}} \in [0,1]$ penalization

$$r_{\mathrm{sym}}(R, \boldsymbol{g}) = \frac{1}{N}\left\| |\mathbf{C}(R)\boldsymbol{g}| - \boldsymbol{g} \right\|_1.$$

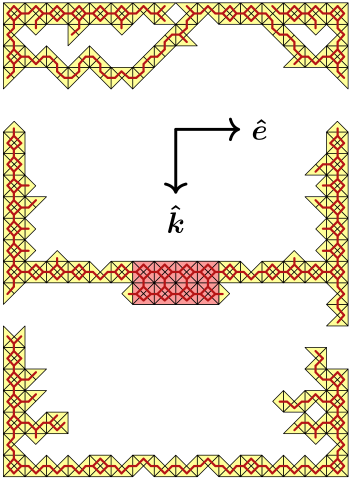
Pareto-type optimization:

$$f(\boldsymbol{g}) = p\left(\mathbf{I}(\boldsymbol{g})\right) + w\, r_{\mathrm{sym}}(\boldsymbol{g}).$$

Concluding Remarks

Geometrical and topological operators

- Powerful and versatile concept.
- Able to deliver manufacture-friendly designs.
- Trade-off between performance and regularity.
- Open ways to combine physics and geometry.



Maximum absorbed power in a chip.

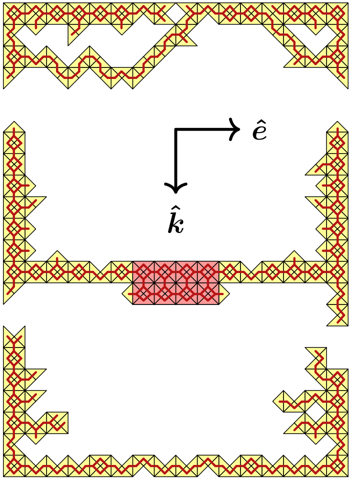
Concluding Remarks

Geometrical and topological operators

- Powerful and versatile concept.
- Able to deliver manufacture-friendly designs.
- Trade-off between performance and regularity.
- Open ways to combine physics and geometry.

Topics of ongoing research

- Synthesis of linear operators.
- What is the best choice of the global scheme?
- What is the best local update strategy?
- Metaparameters have crucial impact on performance.



Maximum absorbed power in a chip.

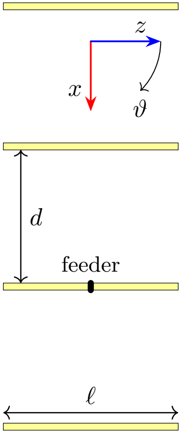
Questions?

Miloslav Čapek
miloslav.capek@fel.cvut.cz

November 23, 2021
version 1.2
The presentation is available at ▶ capek.elmag.org

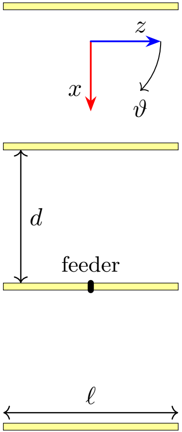
Acknowledgment: This work was supported by the Czech Science Foundation (project No. 19-06049S).

Example #3: Maximal Realized Gain

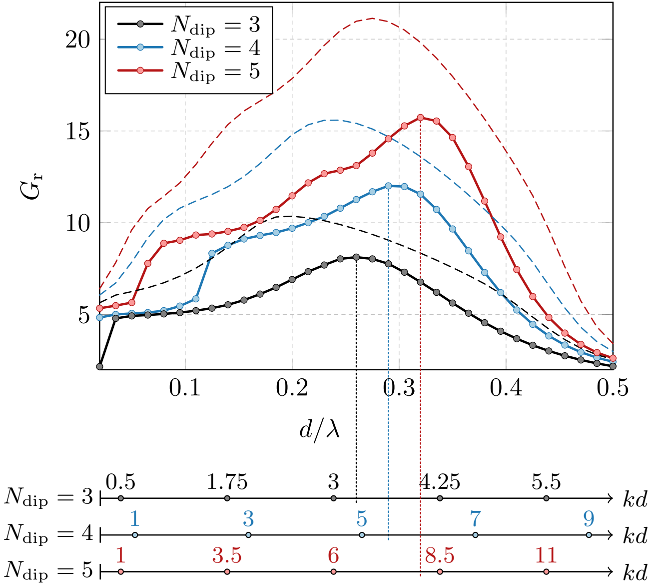


Optimization settings, $N_{\text{dip}} = 4$.

Example #3: Maximal Realized Gain

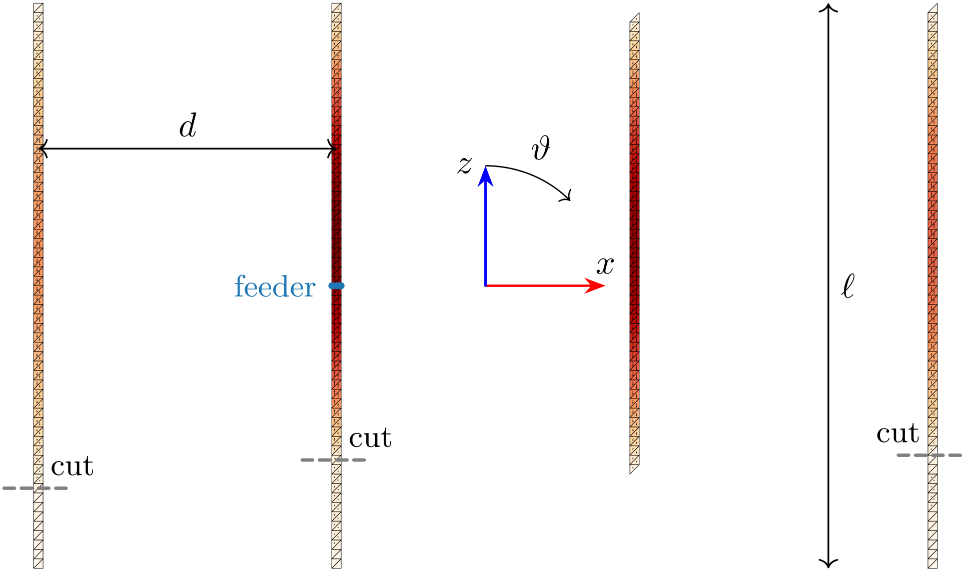


Optimization settings, $N_{\mathrm{dip}} = 4$.



Fundamental bounds (dashed), realized antennas (solid).

Example #3: Maximal Realized Gain (Structure)



1 GHz, copper, $l_{\max} = 0.55\lambda$, $d/\lambda = 0.29$, $Z_0 = 50\,\Omega$, $\hat{\boldsymbol{e}} = \hat{\boldsymbol{z}}$, $\hat{\boldsymbol{d}} = \hat{\boldsymbol{z}}$, $G_{\mathrm{r}} = 12.0$, $G_{\mathrm{r}}^{\mathrm{lb}} = 15.6$.