Fundamental Bounds For Volumetric Structures and Their Feasibility

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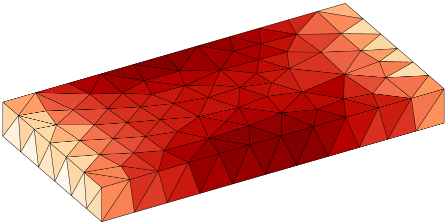
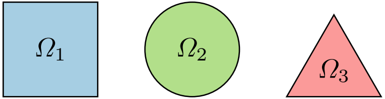
Outline

1. Shape Analysis, Synthesis, and Optimal Design
2. Parameterization of a Model
3. Removal and Addition of DOF
4. Topology Sensitivity for VMoM
5. Topology Sensitivity for VMoM: Examples
6. Concluding Remarks

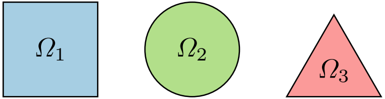


(Sub-)optimal solution of maximum scattering cross section of slab made of gold at 770 MHz.

Analysis × Synthesis



Analysis $\times$ Synthesis



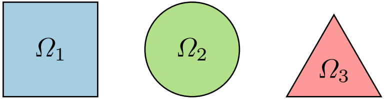
Analysis ($\mathcal{A}$)

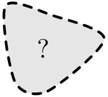
- Shape Ω is given, BCs are known, determine EM quantities.

$$p = \boldsymbol{\mathcal{L}} \boldsymbol{J}(\boldsymbol{r}) = \mathcal{A}\left\{\Omega, \boldsymbol{E}^{\mathrm{i}}\right\}$$

- p is an investigated quantity $(Z_{\mathrm{in}}, Q, P_{\mathrm{rad}}, \eta_{\mathrm{rad}}, \dots)$ or a composite metric

Analysis × Synthesis





Analysis ($\mathcal{A}$)

- Shape Ω is given, BCs are known, determine EM quantities.

$$p = \mathcal{L}\boldsymbol{J}(\boldsymbol{r}) = \mathcal{A}\left\{\Omega, \boldsymbol{E}^{\mathrm{i}}\right\}$$

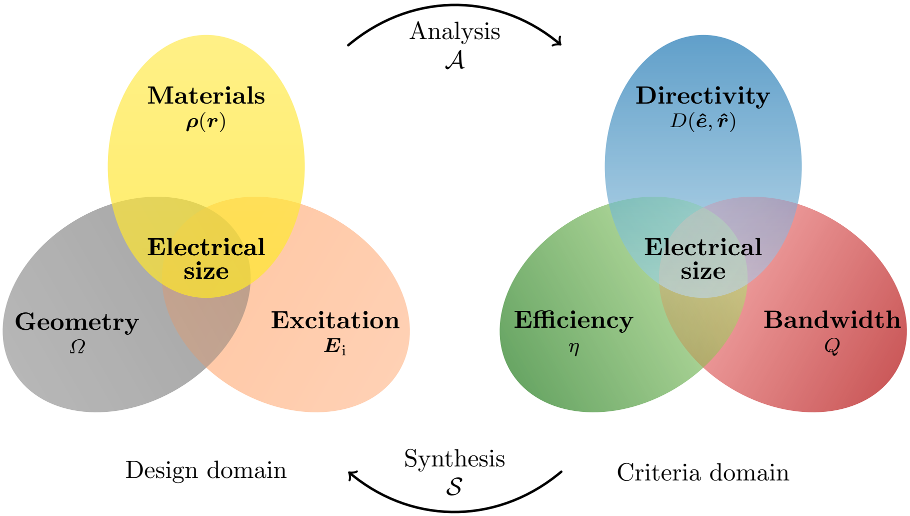
Synthesis ($\mathcal{S} \equiv \mathcal{A}^{-1}$)

- EM behavior is specified, neither Ω nor BCs are known.

$$\left\{\Omega, \boldsymbol{E}^{\mathrm{i}}\right\} = \mathcal{A}^{-1} p = \mathcal{S} p$$

- p is an investigated quantity (Z_{in}, Q, P_{rad}, $\eta_{\mathrm{rad}}, \dots$) or a composite metric

Antenna Design



Shape Synthesis: Rigorous Definition

For a given impedance matrix $\mathbf{Z} \in \mathbb{C}^{N\times N}$, matrices $\mathbf{A}$, $\{\mathbf{B}_i\}$, $\{\mathbf{B}_j\}$, (a given) excitation vector $\mathbf{V} \in \mathbb{C}^N$, find a vector $\boldsymbol{x}$ such that

$$\begin{aligned} \text{minimize} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{A}\left(\boldsymbol{x}\right) \mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{B}_i\left(\boldsymbol{x}\right) \mathbf{I} = p_i \\ & \mathbf{I}^{\mathrm{H}} \mathbf{B}_j\left(\boldsymbol{x}\right) \mathbf{I} \leq p_j \\ & \mathbf{Z}\left(\boldsymbol{x}\right) \mathbf{I} = \mathbf{V} \\ & \boldsymbol{x} \in \{0,1\}^N \end{aligned}$$

$$\boldsymbol{x} = \begin{bmatrix} 1 & 1 & 0 & \cdots & 1 \end{bmatrix}$$

$$\begin{bmatrix} Z_{11} & Z_{12} & Z_{13} & \cdots & Z_{1N} \\ Z_{21} & Z_{22} & Z_{23} & \cdots & Z_{2N} \\ Z_{31} & Z_{32} & Z_{33} & \cdots & Z_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ Z_{N1} & Z_{N2} & Z_{N3} & \cdots & Z_{NN} \end{bmatrix} \begin{bmatrix} I_1 \\ I_2 \\ I_3 \\ \vdots \\ I_N \end{bmatrix} = \begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ \vdots \\ V_N \end{bmatrix}$$

[1] G. L. Nemhauser and L. A. Wolsey, *Integer an Combinatorial Optimization*. John Wiley & Sons, 1999, ISBN: 0-471-35943-2

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- Combinatorial optimization[1] (suffers from curse of dimensionality, 2^N possible solutions),
- vector $\boldsymbol{x}$ serves as a characteristic function (structure perturbation).

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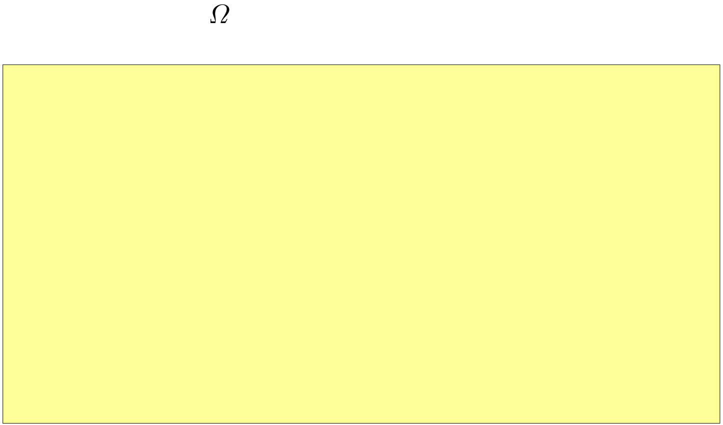
Degrees of Freedom

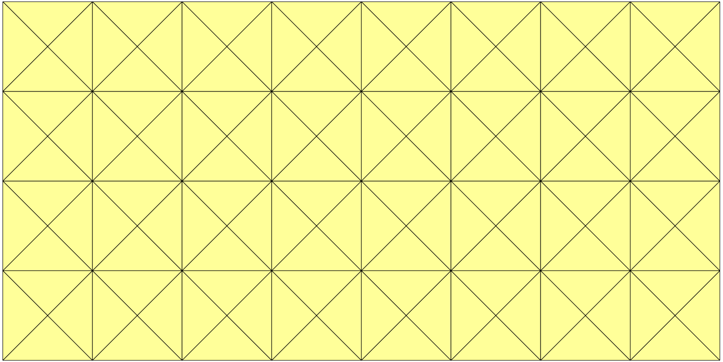
Bounding box



Degrees of Freedom

Bounding box→ discretization

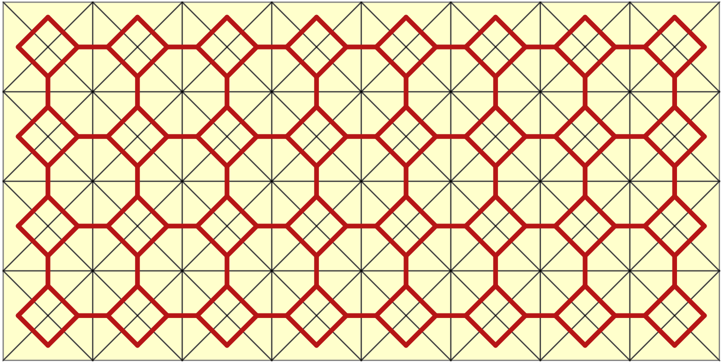
$$\Omega \to \{T_t\}$$



Degrees of Freedom

Bounding box→ discretization→ basis functions

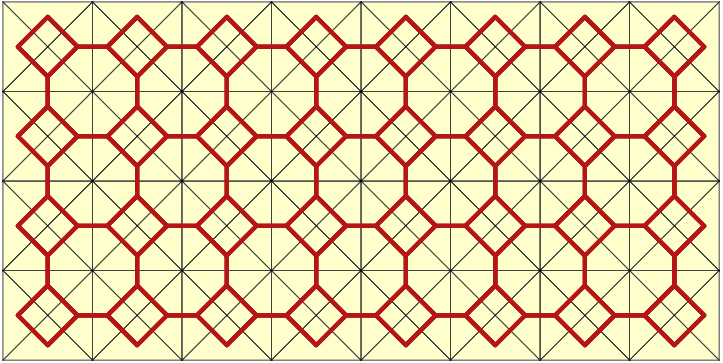
$$\Omega \rightarrow \{T_t\} \rightarrow \{\boldsymbol{\psi}_n(\boldsymbol{r})\}$$



Degrees of Freedom

Bounding box→ discretization→ basis functions→ degrees of freedom to be optimized

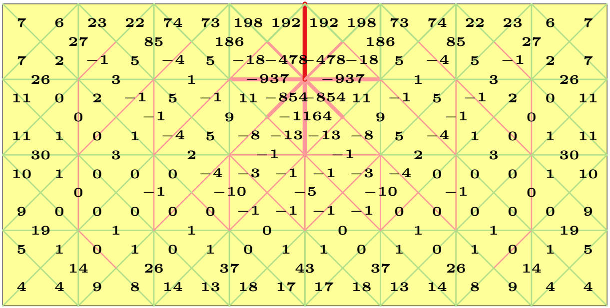
$$\Omega \to \{T_t\} \to \{\boldsymbol{\psi}_n(\boldsymbol{r})\} \to \boldsymbol{g}$$



- $\mathbf{g} \in \{0,1\}^{N\times 1}$ is characteristic vector (discretized characteristic function)

Shape Optimization With Exact Reanalysis

Capability to effectively remove/add a degree of freedom.[2]

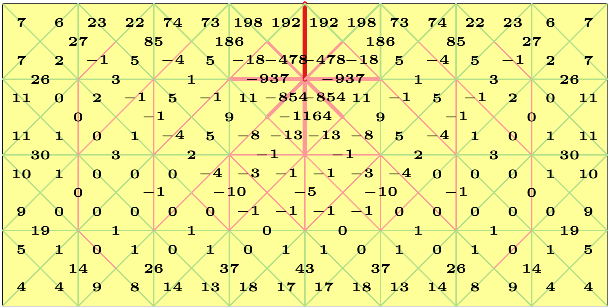


[2] M. Capek, L. Jelinek, and M. Gustafsson, “Shape synthesis based on topology sensitivity,” *IEEE Trans. Antennas Propag.*, vol. 67, no. 6, pp. 3889 –3901, 2019. DOI: 10.1109/TAP.2019.2902749

Shape Optimization With Exact Reanalysis

Capability to effectively remove/add a degree of freedom.[2]

- Perfectly compatible with method of moments;
  - basis functions used as DOF.



Example of topology sensitivity, $ka = 1/2$, plate fed in the middle.

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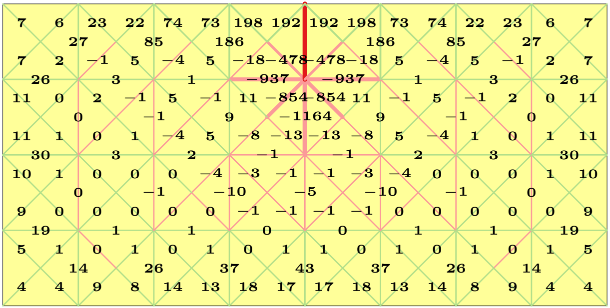
Shape Optimization With Exact Reanalysis

Capability to effectively remove/add a degree of freedom.[2]

- Perfectly compatible with method of moments;
  - basis functions used as DOF.
- Inversion-free for the smallest perturbations;
  - gradient-based shape optimization possible deterministically.



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Update of an EM System With Exact Reanalysis

Modification of the shape described by impedance matrix $\mathbf{Z}$

$$\mathbf{Y} = \mathbf{Z}^{-1} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} = \begin{bmatrix} \mathbf{A}^{-1} + \mathbf{A}^{-1}\mathbf{B}\mathbf{E}^{-1}\mathbf{C}\mathbf{A}^{-1} & -\mathbf{A}^{-1}\mathbf{B}\mathbf{E}^{-1} \\ -\mathbf{E}^{-1}\mathbf{C}\mathbf{A}^{-1} & \mathbf{E}^{-1} \end{bmatrix}$$

and consequently perturbation of the current density

$$\mathbf{I} = \mathbf{Y}\mathbf{V}. \tag{1}$$

Removing and Adding DOF (Delta Gap Feeder)

DOF removal:

$$\widehat{\mathbf{I}} = \left(\mathbf{y}_f - \frac{Y_{fb}}{Y_{bb}}\mathbf{y}_b\right) l_f V_0,$$

Admittance matrix update:

$$\widehat{\mathbf{Y}} = \mathbf{C}^{\mathrm{T}} \left(\mathbf{Y} - \frac{1}{Y_{bb}}\mathbf{y}_b\mathbf{y}_b^{\mathrm{T}}\right) \mathbf{C},$$

DOF addition:

$$\widehat{\mathbf{I}} = \mathbf{C}^{\mathrm{T}} \left(\begin{bmatrix} \mathbf{y}_f \\ 0 \end{bmatrix} + \frac{x_{fb}}{z_b}\begin{bmatrix} \mathbf{x}_b \\ -1 \end{bmatrix}\right) l_f V_0,$$

Admittance matrix update:

$$\widehat{\mathbf{Y}} = \frac{1}{z_b}\mathbf{C}^{\mathrm{T}} \begin{bmatrix} z_b\mathbf{Y} + \mathbf{x}_b\mathbf{x}_b^{\mathrm{T}} & -\mathbf{x}_b \\ -\mathbf{x}_b^{\mathrm{T}} & 1 \end{bmatrix} \mathbf{C},$$

$$C_{nn} = \begin{cases} 0 & \Leftrightarrow \quad g_n = b \\ 1 & \Leftrightarrow \quad \text{otherwise} \end{cases}$$

$$\mathbf{x}_b = \mathbf{Y}\widetilde{\mathbf{z}}_b, \quad z_b = \widetilde{Z}_{bb} - \widetilde{\mathbf{z}}_b^{\mathrm{T}}\mathbf{x}_b$$

$$C_{mn} = \begin{cases} 1 & \Leftrightarrow \quad g_n = S(m) \\ 0 & \Leftrightarrow \quad \text{otherwise} \end{cases}$$

- All columns of **C** matrix containing solely zeros are eliminated before use.

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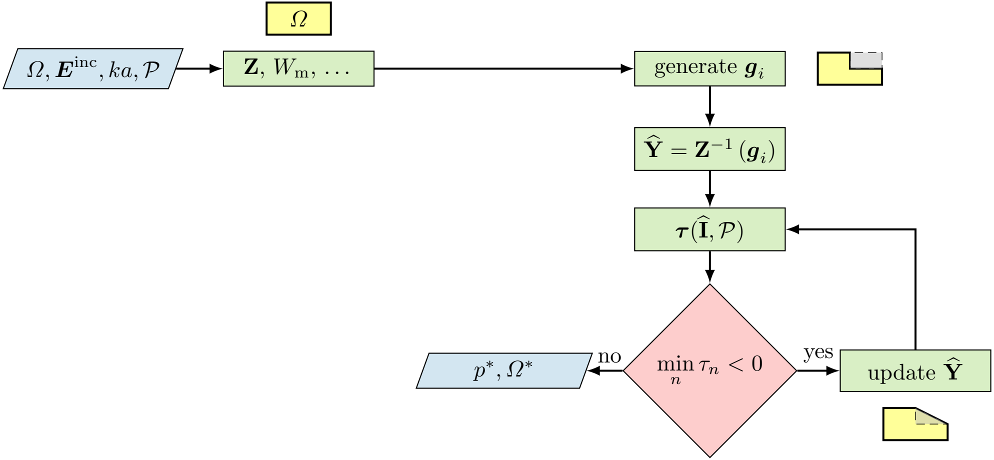
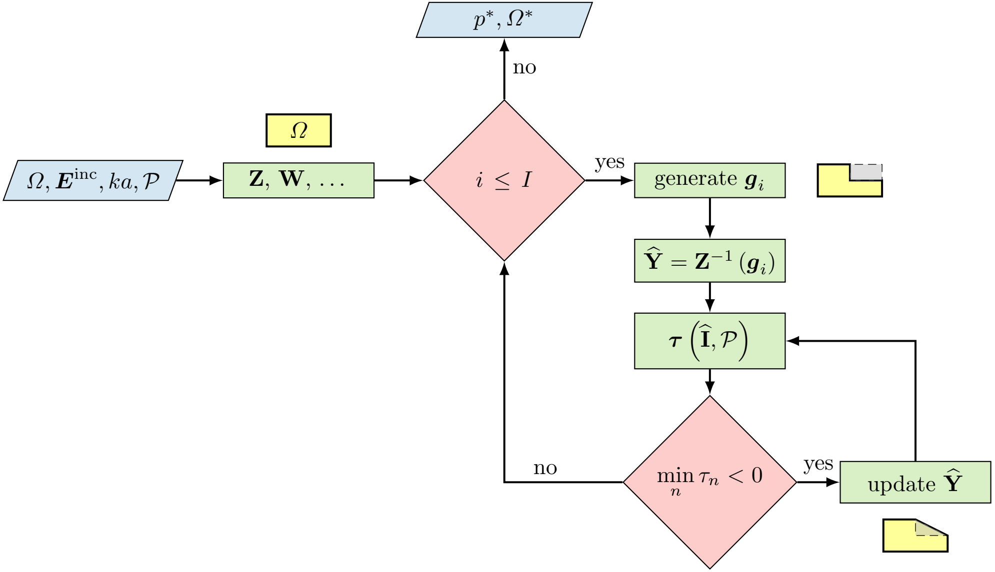
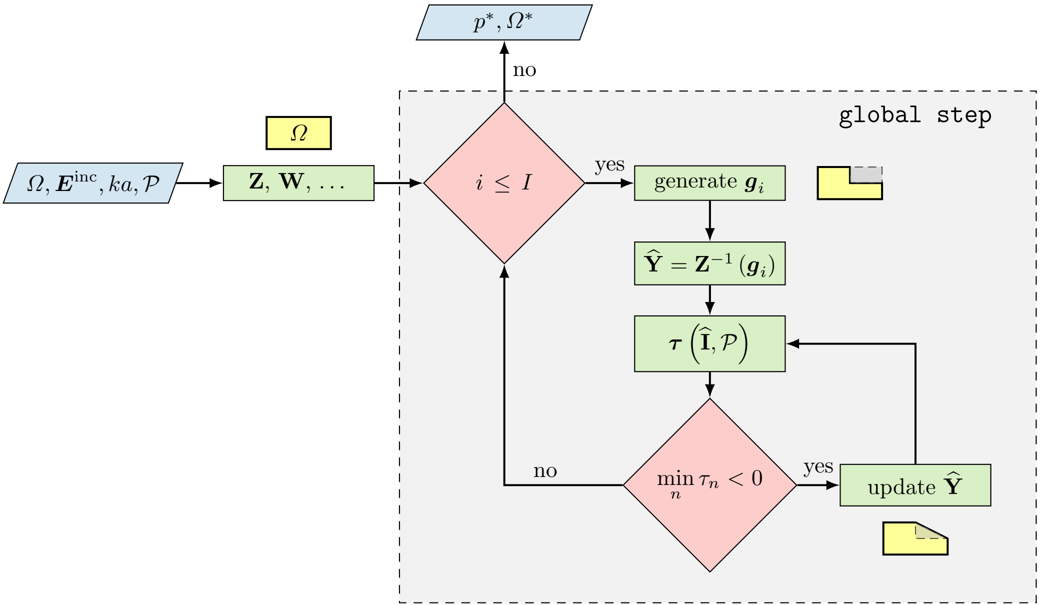

Ω
$\Omega, \boldsymbol{E}^{\mathrm{inc}}, ka, \mathcal{P}$
$\mathbf{Z}, W_{\mathrm{m}}, \dots$
generate $\boldsymbol{g}_i$
$\widehat{\mathbf{Y}} = \mathbf{Z}^{-1}(\boldsymbol{g}_i)$
$\boldsymbol{\tau}(\widehat{\mathbf{I}}, \mathcal{P})$
$\min_n \tau_n < 0$
no
yes
p^*, Ω^*
update $\widehat{\mathbf{Y}}$


$p^*, \mathit{\Omega}^*$
no
$\mathit{\Omega}$
$\mathit{\Omega}, \boldsymbol{E}^{\mathrm{inc}}, ka, \mathcal{P}$
$\mathbf{Z}, \mathbf{W}, \ldots$
$i \leq I$
yes
generate $\boldsymbol{g}_i$
$\widehat{\mathbf{Y}} = \mathbf{Z}^{-1}(\boldsymbol{g}_i)$
$\boldsymbol{\tau}\left(\widehat{\mathbf{I}}, \mathcal{P}\right)$
no
$\min\limits_n \tau_n < 0$
yes
update $\widehat{\mathbf{Y}}$


p^*, Ω^*
no
global step
Ω
$\Omega, \boldsymbol{E}^{\mathrm{inc}}, ka, \mathcal{P}$
$\mathbf{Z}, \mathbf{W}, \dots$
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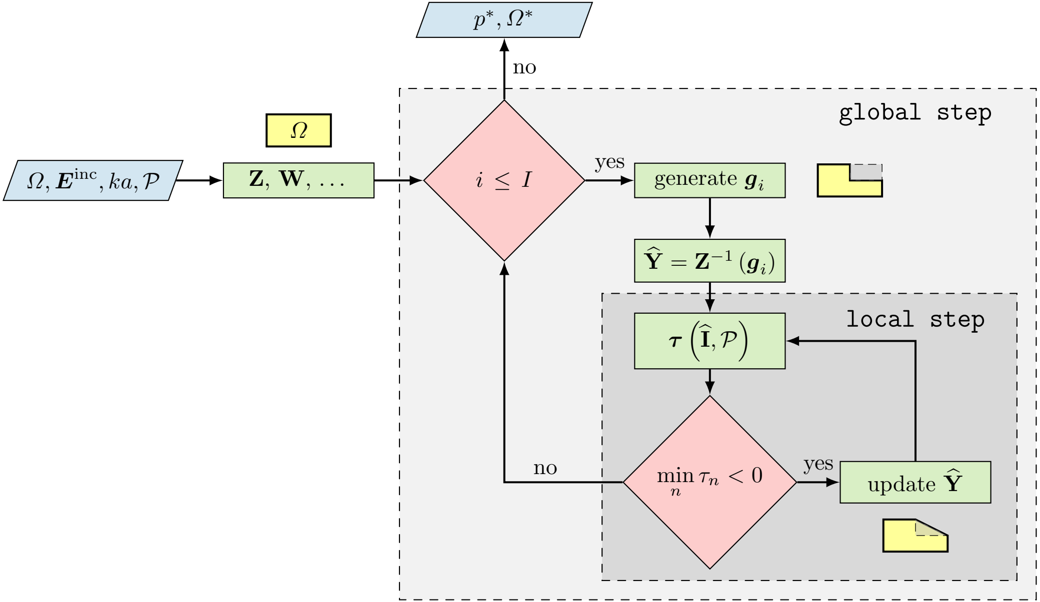
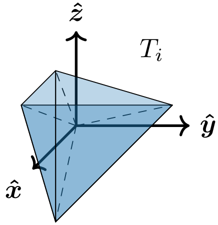
no
$\min_n \tau_n < 0$
yes
update $\widehat{\mathbf{Y}}$


p^*, Ω^*
no
global step
Ω
$\Omega, \boldsymbol{E}^{\mathrm{inc}}, ka, \mathcal{P}$
$\mathbf{Z}$, $\mathbf{W}$, ...
$i \leq I$
yes
generate $\boldsymbol{g}_i$
$\widehat{\mathbf{Y}} = \mathbf{Z}^{-1}(\boldsymbol{g}_i)$
local step
$\boldsymbol{\tau}\left(\widehat{\mathbf{I}}, \mathcal{P}\right)$
no
$\min_n \tau_n < 0$
yes
update $\widehat{\mathbf{Y}}$

Volumetric Method of Moments

- Tetrahedral discretization.
- Piece-wise constant basis functions.
- (Expensive) volumetric quadrature converted to surface integrals [3].



$$Z_{mn} = -\mathrm{j}\frac{Z_0}{k}\int\limits_{V_m} \boldsymbol{\psi}_m(\boldsymbol{r}) \cdot \left(\mathbf{1} + \boldsymbol{\chi}^{-1}(\boldsymbol{r})\right) \cdot \boldsymbol{\psi}_n(\boldsymbol{r}) \,\mathrm{d}V - \mathrm{j}\frac{Z_0}{k}\oint\limits_{S_m}\oint\limits_{S_n} \Psi_{mn}(\boldsymbol{r},\boldsymbol{r}') G(\boldsymbol{r},\boldsymbol{r}') \,\mathrm{d}S'\,\mathrm{d}S,$$

$$\Psi_{mn}(\boldsymbol{r},\boldsymbol{r}') = \boldsymbol{\psi}_m(\boldsymbol{r}) \cdot \boldsymbol{n}_n(\boldsymbol{r}')\,\boldsymbol{\psi}_n(\boldsymbol{r}') \cdot \boldsymbol{n}_m(\boldsymbol{r}) - \boldsymbol{\psi}_m(\boldsymbol{r}) \cdot \boldsymbol{\psi}_n(\boldsymbol{r}')\,\boldsymbol{n}_n(\boldsymbol{r}') \cdot \boldsymbol{n}_m(\boldsymbol{r})$$

[3] A. Polimeridis, J. Villena, L. Daniel, *et al.*, "Stable FFT-JVIE solvers for fast analysis of highly inhomogeneous dielectric objects," *Journal of Computational Physics*, vol. 269, pp. 280–296, 2014. DOI: 10.1016/j.jcp.2014.03.026. [Online]. Available: https://doi.org/10.1016/j.jcp.2014.03.026

Radiation Efficiency Bounds

- The optimization problems $\mathcal{P}_1$ and $\mathcal{P}_2$ can rigorously be formulated.

Maximum radiation efficiency

Problem $\mathcal{P}_1$:

$$\begin{aligned} \text{minimize} \quad & P_{\text{loss}} \\ \text{subject to} \quad & P_{\text{rad}} = 1 \end{aligned}$$

Maximum self-resonant radiation efficiency

Problem $\mathcal{P}_2$:

$$\begin{aligned} \text{minimize} \quad & P_{\text{loss}} \\ \text{subject to} \quad & P_{\text{rad}} = 1 \\ & \omega \left(W_{\text{m}} - W_{\text{e}} \right) = 0 \end{aligned}$$

Radiation Efficiency Bounds

- The optimization problems $\mathcal{P}_1$ and $\mathcal{P}_2$ can rigorously be formulated.
- Having quadratic forms for the physical quantities, the antenna metrics may be optimized.

Maximum radiation efficiency

Problem $\mathcal{P}_1$:

$$\begin{aligned} \text{minimize} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_\rho \mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_0 \mathbf{I} = 1 \end{aligned}$$

Maximum self-resonant radiation efficiency

Problem $\mathcal{P}_2$:

$$\begin{aligned} \text{minimize} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_\rho \mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_0 \mathbf{I} = 1 \\ & \mathbf{I}^{\mathrm{H}} \mathbf{X} \mathbf{I} = 0 \end{aligned}$$

Radiation Efficiency Bounds

- The optimization problems $\mathcal{P}_1$ and $\mathcal{P}_2$ can rigorously be formulated.
- Having quadratic forms for the physical quantities, the antenna metrics may be optimized.
- The problems $\mathcal{P}_1$ and $\mathcal{P}_2$ are quadratically constrained quadratic programs[4] (QCQP).

Maximum radiation efficiency

Problem $\mathcal{P}_1$:

$$\begin{aligned} \text{minimize} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_\rho \mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_0 \mathbf{I} = 1 \end{aligned}$$

Maximum self-resonant radiation efficiency

Problem $\mathcal{P}_2$:

$$\begin{aligned} \text{minimize} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_\rho \mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathrm{H}} \mathbf{R}_0 \mathbf{I} = 1 \\ & \mathbf{I}^{\mathrm{H}} \mathbf{X} \mathbf{I} = 0 \end{aligned}$$

Algebraic Representation of Integral Operators

Radiated and reactive power

Complex power balance:

$$P_{\mathrm{rad}} + P_{\mathrm{lost}} + 2\mathrm{j}\omega \left(W_{\mathrm{m}} - W_{\mathrm{e}} \right) = \frac{1}{2} \langle \boldsymbol{J}\left(\boldsymbol{r}\right), \mathcal{Z}\left[\boldsymbol{J}\left(\boldsymbol{r}\right)\right] \rangle \approx \frac{1}{2} \mathbf{I}^{\mathrm{H}} \mathbf{Z} \mathbf{I} \qquad (2)$$

Radiated power:

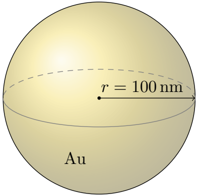
$$P_{\mathrm{rad}} \approx \frac{1}{2} \mathbf{I}^{\mathrm{H}} \mathbf{R}_0 \mathbf{I} \qquad (3)$$

Lost power:

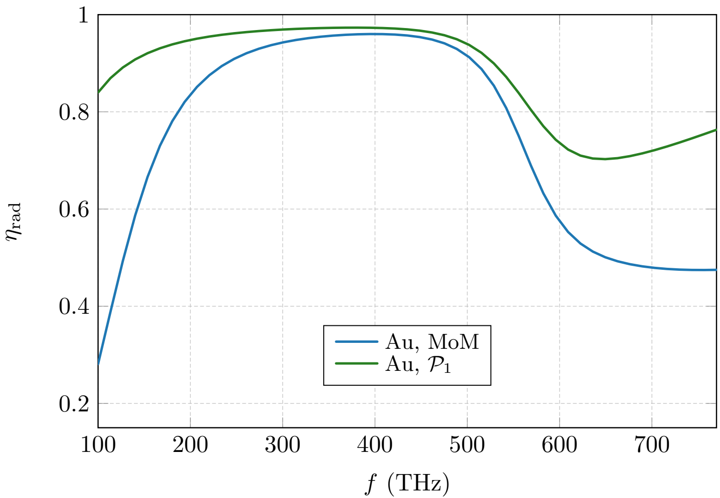
$$P_{\mathrm{lost}} \approx \frac{1}{2} \mathbf{I}^{\mathrm{H}} \mathbf{R}_\rho \mathbf{I} \qquad (4)$$

$$Z_{mn} = -\mathrm{j} \frac{Z_0}{k} \int\limits_{V_m} \boldsymbol{\psi}_m\left(\boldsymbol{r}\right) \cdot \left(\mathbf{1} + \boldsymbol{\chi}^{-1}\left(\boldsymbol{r}\right)\right) \cdot \boldsymbol{\psi}_n\left(\boldsymbol{r}\right) \, \mathrm{d}V - \mathrm{j} \frac{Z_0}{k} \oint\limits_{S_m} \oint\limits_{S_n} \Psi_{mn}(\boldsymbol{r}, \boldsymbol{r}') G\left(\boldsymbol{r}, \boldsymbol{r}'\right) \, \mathrm{d}S' \, \mathrm{d}S,$$

Example: A Gold Nanoparticle – Radiation Efficiency



A particle (Au).



Radiation efficiency: MoM solution compared with optimal performance.

Scattering Cross Section in Dielectric Slab

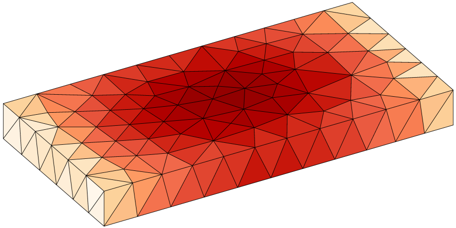
Fundamental bound[5]:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{I}^{\mathrm{H}}\mathbf{R}_0\mathbf{I} \\ \text{subject to} \quad & \mathbf{I}^{\mathrm{H}}\mathbf{R}\mathbf{I} - \mathrm{Re}\{\mathbf{I}^{\mathrm{H}}\mathbf{V}\} = 0 \\ & \mathbf{I}^{\mathrm{H}}\mathbf{X}\mathbf{I} - \mathrm{Im}\{\mathbf{I}^{\mathrm{H}}\mathbf{V}\} = 0 \end{aligned}$$

MoM evaluation (for topology optimization):

$$\mathbf{I} = \mathbf{Z}^{-1}\mathbf{V}$$

$$\sigma_{\mathrm{scat}} = \frac{1}{2}\frac{\mathbf{I}^{\mathrm{H}}\mathbf{R}_0\mathbf{I}}{S_0}$$

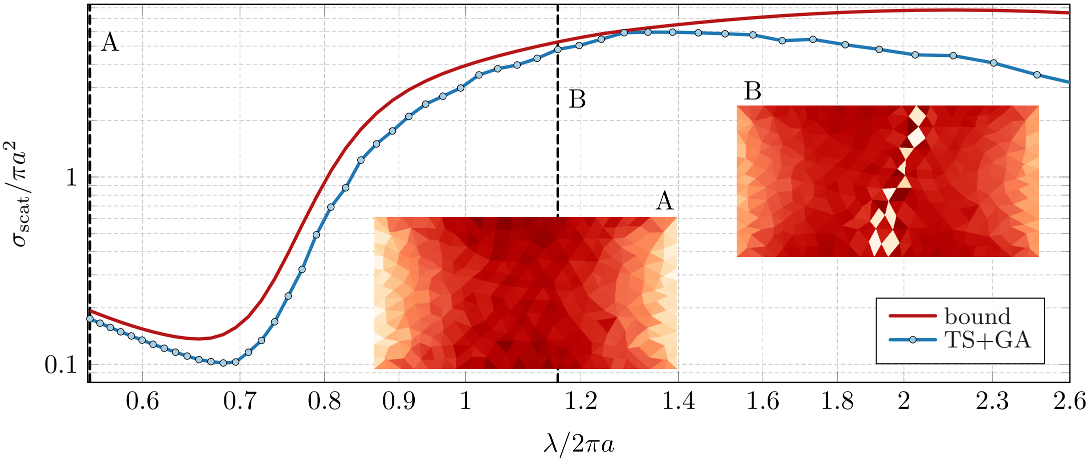


Optimal current maximizing scattering cross section at 770 MHz, VMoM, golden slab.

[5] M. Gustafsson, K. Schab, L. Jelinek, *et al.*, "Upper bounds on absorption and scattering,", 2019, eprint arXiv: 1912.06699. [Online]. Available: https://arxiv.org/abs/1912.06699

[6] A. Derkachova, K. Kolwas, and I. Demchenko, "Dielectric function for gold in plasmonics applications: Size dependence of plasmon resonance frequencies and damping rates for nanospheres," *Plasmonics*, vol. 11, pp. 941–951, 3 Jun. 2016. DOI: 10.1007/s11468-015-0128-7

Comparison of Fundamental Bounds and Optimal Designs



Optimization setting: slab $\ell \times \ell/2 \times \ell/10$, $\ell = 200\,\mathrm{nm}$, $f \in [160, 770]\,\mathrm{THz}$, gold[6], plane wave ($\mathbf{V}$) polarized along $\boldsymbol{x}$ axis, perpendicular angle of incidence, 1380 basis functions.

Concluding Remarks

What has been done

- Deterministic inversion-free structure perturbation (removal/addition).
- A novel memetic algorithm.
- Knowledge of gradients for a given (fixed) EM model.
- Robustness and immunity against local minima.

Concluding Remarks

What has been done

- Deterministic inversion-free structure perturbation (removal/addition).
- A novel memetic algorithm.
- Knowledge of gradients for a given (fixed) EM model.
- Robustness and immunity against local minima.

Topics of ongoing research

- Acceleration on GPUs.
- Utilization of big data gathered during the optimization.
- Regularization to remove irregularities.
- Adaptive Greedy strategies to overcome slow convergence.
- How to interpret enabled/disabled $\{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}$ basis functions? Anisotropic material?

Questions?

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version 1.0
The presentation is available at ▶ capek.elmag.org

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