Optimal Absorption & Scattering in Embedded Design Problems

Kurt Schab[1], **Austin Rothschild*[1]**, Miloslav Capek[2], Lukas Jelinek[2], and Mats Gustafsson[3]

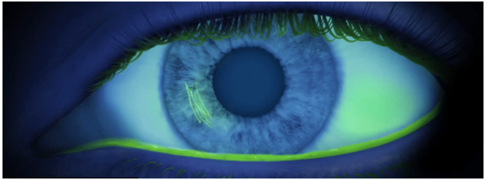
[1]Santa Clara University, USA
[2]Czech Technical University in Prague, Czech Republic
[3]Lund University, Sweden

March 26, 2021

Outline

Background: Nanophotonics, fundamental bounds, & inverse design

- *Nanophotonics:* study of light-matter interactions on the nanometer scale
- **Applications**
  - Fluorescence
  - Near-field & on-chip optics
  - Photonic crystals
- *Fundamental bound:* absolute limit on system performance subject to constraints
- *Inverse design:* using optimization to search for device with best performance
- Fundamental bounds give insight into performance characteristics devices can reach via inverse design



Source: *rebelem.com*

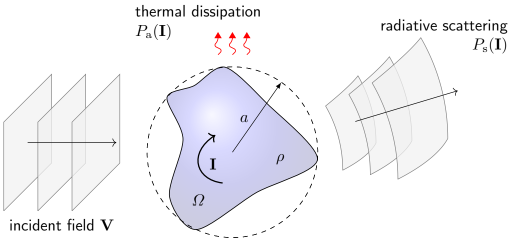
Background: History, Development, & Techniques

- **Recent efforts:** *finding physical bounds on performance parameters of plasmonic and photonic devices*
  - Cross-section bounds; directional scattering
  - Radiative heat transfer
  - Near-field enhancement/Purcell factor
- **Order of development:**
  - Shape-independent bounds **[Miller et al. 2016]**
  - Shape-dependent bounds **[Molesky et al. 2020]**
  - Shape & material-dependent bounds **[Gustafsson, Schab, Jelinek, & Capek 2020]**
- Strategies for deriving bounds on performance for microwave antennas (efficiency, directivity, Q-factor) can be reformulated to analyze problems in nanophotonics

Background: Scattering, Absorption, and Extinction

- Qualify nanophotonic structures with:
  - $P_{\mathrm{a}}(\mathbf{I})$, **Absorbed power:** Total cycle-mean power dissipated by an arbitrary current $\mathbf{I}$. Dependent on material.
  - $P_{\mathrm{s}}(\mathbf{I})$, **Scattered power:** Total cycle-mean power radiated by $\mathbf{I}$. Dependent on free-space.
  - $P_{\mathrm{t}}(\mathbf{I}, \mathbf{V})$, **Extincted power:** Sum of $P_{\mathrm{a}} + P_{\mathrm{s}}$

$$\begin{aligned} \mathbf{V} = \mathbf{Z}\mathbf{I} &= (\mathbf{R} + \mathrm{i}\mathbf{X})\,\mathbf{I} \\ \mathbf{R} &= \mathbf{R}_0 + \mathbf{R}_\rho \\ \mathbf{X} &= \mathbf{X}_0 + \mathbf{X}_\rho \end{aligned}$$



Goal

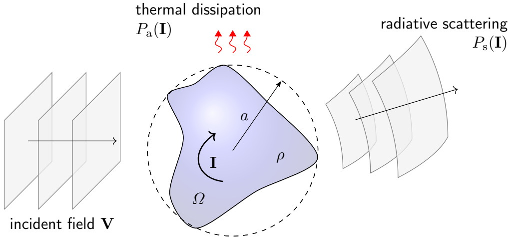
Study "best possible" limits of scattering, absorption, and extinction cross-sections for an object of arbitrary shape and material properties.

Outline

Current-Based Optimization Problems

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

- satisfies Maxwell's equations
- unique
- implies specific structure within Ω



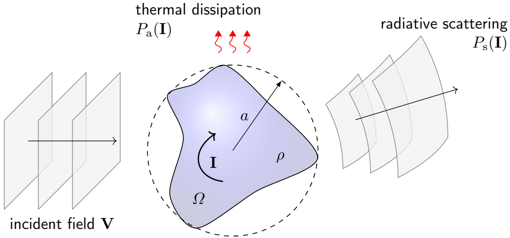
Current-Based Optimization Problems

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

- satisfies Maxwell's equations
- unique
- implies specific structure within Ω

Relaxed solutions: $\{\mathbf{I} : \mathbf{I}^{\mathrm{H}}\mathbf{Z}\mathbf{I} = \mathbf{I}^{\mathrm{H}}\mathbf{V}\}$

- satisfies global power conservation
- non-unique
- contains driven currents on all possible substructures within Ω



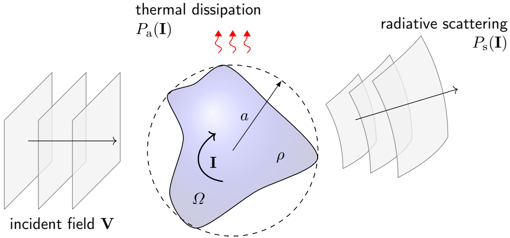
Current-Based Optimization Problems

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

- satisfies Maxwell's equations
- unique
- implies specific structure within Ω

Relaxed solutions: $\{\mathbf{I} : \mathbf{I}^{\mathrm{H}}\mathbf{Z}\mathbf{I} = \mathbf{I}^{\mathrm{H}}\mathbf{V}\}$

- satisfies global power conservation
- non-unique
- contains driven currents on all possible substructures within Ω



Strategy

Form optimization problems over all relaxed solutions to find performance bounds

$$\max_{\mathbf{I}} \; C(\mathbf{I}), \quad \text{s.t. } \mathbf{I}^{\mathrm{H}}\mathbf{Z}\mathbf{I} = \mathbf{I}^{\mathrm{H}}\mathbf{V}$$

General Optimization Procedure: Multiple Objectives

$$\begin{aligned} \max \quad & w_{\mathrm{a}} P_{\mathrm{a}} + w_{\mathrm{s}} P_{\mathrm{s}} \\ \text{s.t.} \quad & P_{\mathrm{a}} + P_{\mathrm{s}} - P_{\mathrm{t}} = 0, \end{aligned}$$

$$\begin{aligned} \max_{\mathbf{I}} \quad & \mathbf{I}^{\mathrm{H}}(w_{\mathrm{a}}\mathbf{R}_{\rho} + w_{\mathrm{s}}\mathbf{R}_0)\mathbf{I} \\ \text{s.t.} \quad & \mathbf{I}^{\mathrm{H}}(\mathbf{R}_{\rho} + \mathbf{R}_0)\mathbf{I} - \mathrm{Re}\{\mathbf{I}^{\mathrm{H}}\mathbf{V}\} = 0. \end{aligned}$$

A way to study the relative *trade-off* between conflicting goals by assigning arbitrary weights to a given objective.

No single solution exists that simultaneously optimizes each objective.

- Multi-objective problem yields a *Pareto-optimal* set: set of points at which an increase in performance in one parameter must be accompanied by performance decrease in the other.
- Feasible solution space is visualized by the Pareto-frontier.

Simultaneous Maximization

$$\begin{aligned} \max_{\mathbf{I}} \quad & \alpha P_{\mathrm{a}} + (1-\alpha) P_{\mathrm{s}} \\ \text{s.t.} \quad & P_{\mathrm{a}} + P_{\mathrm{s}} - P_{\mathrm{t}} = 0 \end{aligned}$$

$$\begin{aligned} \max_{\mathbf{I}} \quad & \alpha \mathbf{I}^{\mathrm{H}} \mathbf{R}_{\rho} \mathbf{I} + (1-\alpha) \mathbf{I}^{\mathrm{H}} \mathbf{R}_{0} \mathbf{I} \\ \text{s.t.} \quad & \mathbf{I}^{\mathrm{H}} (\mathbf{R}_{\rho} + \mathbf{R}_{0}) \mathbf{I} - \mathrm{Re}\{\mathbf{I}^{\mathrm{H}} \mathbf{V}\} = 0 \end{aligned}$$

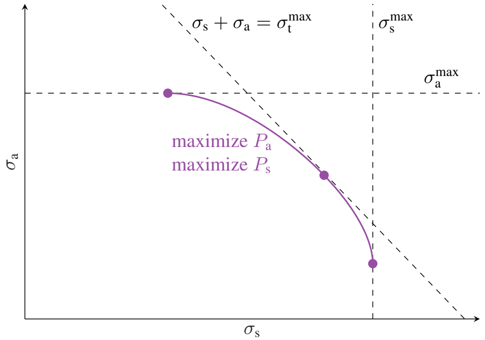
- *Goal*: maximize absorbed and scattered power with regards to conservation of power
  - What is trade-off between maximized absorption and scattering?
- Objective functions are weighted such that $w_{\mathrm{a}} = \alpha$, $w_{\mathrm{s}} = (1-\alpha)$ for $\alpha \in [0,1]$
  - $\alpha = 1$ $\rightarrow$ maximum absorption
  - $\alpha = 0$ $\rightarrow$ maximum scattering
  - $\alpha = 0.5$ $\rightarrow$ maximum extincted power

Simultaneous maximization

$$\max_{\mathbf{I}} \quad \alpha \mathbf{I}^{\mathrm{H}} \mathbf{R}_\rho \mathbf{I} + (1-\alpha) \mathbf{I}^{\mathrm{H}} \mathbf{R}_0 \mathbf{I}$$

$$\text{s.t.} \quad \mathbf{I}^{\mathrm{H}} (\mathbf{R}_\rho + \mathbf{R}_0) \mathbf{I} - \mathrm{Re}\{\mathbf{I}^{\mathrm{H}} \mathbf{V}\} = 0$$

$$\alpha \in [0, 1]$$

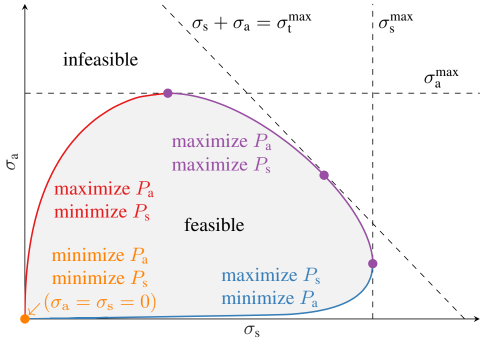


Simultaneous maximization Pareto front for fixed ka and real resistivity $\rho_r/a\ \Omega$.

Extending the Weights

$$\begin{aligned} \max_{\mathbf{I}} \quad & \mathbf{I}^{\mathrm{H}}(w_{\mathrm{a}}\mathbf{R}_\rho + w_{\mathrm{s}}\mathbf{R}_0)\mathbf{I} \\ \text{s.t.} \quad & \mathbf{I}^{\mathrm{H}}(\mathbf{R}_\rho + \mathbf{R}_0)\mathbf{I} - \mathrm{Re}\{\mathbf{I}^{\mathrm{H}}\mathbf{V}\} = 0 \\ & w_{\mathrm{a}} = \cos\phi, w_{\mathrm{s}} = \sin\phi \\ & \phi \in [0, 2\pi] \end{aligned}$$

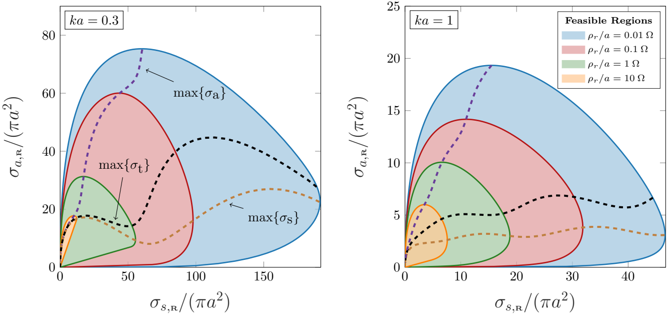
- Weight extension considers three additional optimization problems
  1. max P_{a}, min P_{s}
  2. max P_{s}, min P_{a}
  3. min P_{s}, min P_{a}
- Union of all problems (arbitrary real weights) leads to the *closed feasible region*



Union of 4-separate optimization problems for absorption/scattering results in closed-feasible region for an object confined to electrical size ka.

Closed Feasible Regions: Examples

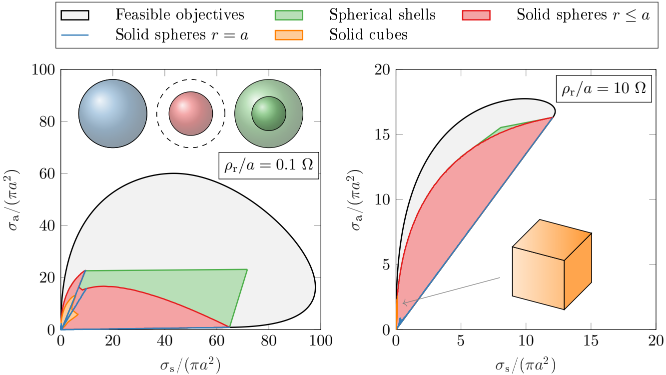
- Holding ka fixed and sweeping over different fixed real resistivities ρ_r generates multiple closed Pareto fronts
- Size of the feasible objective space depends on *material* and *geometry*



Feasible sets on $\sigma_{s,\mathrm{R}}/(\pi a^2)$, $\sigma_{a,\mathrm{R}}/(\pi a^2)$ for obstacles composed of a material with $\rho_r/a \in \{0.01, 0.1, 1, 10\}\,\Omega$ circumscribed by spheres with radii $ka = 0.3$ (left), and $ka = 1$ (right).

Are the bounds tight? Filling the Closed Feasible Regions

- Feasible solution region (gray), realized solutions (blue, red, green)
- **Blue:** solid spheres, $r = a$, parameterized imaginary resistivity ρ_{i}
- **Red:** solid spheres, $r \leq a$, parameterized ρ_{i}
- **Green:** core-shell, fixed core radius $r' = a/2$, independent variation of ρ_{i} in core/shell layers



Realized cross-sections for designs confined to a sphere of size $ka = 0.3$ with fixed real resistivity $\rho_{\mathrm{r}}/a = 0.1\ \Omega$ (left) and $\rho_{\mathrm{r}}/a = 10\ \Omega$ (right).

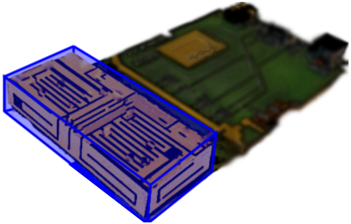
Outline

Application: Embedded Design Problems

- *Embedded design:* devices containing separate regions, with only specified regions able to be altered

Application: Embedded Design Problems

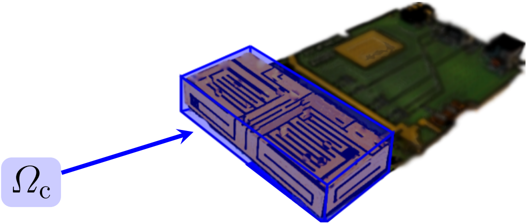
- *Embedded design:* devices containing separate regions, with only specified regions able to be altered
- **Example**
  - Chassis (vehicle) mounted antennas



[Gustafsson, 2016]

Application: Embedded Design Problems

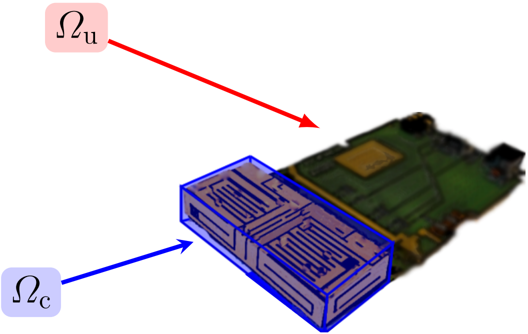
- *Embedded design:* devices containing separate regions, with only specified regions able to be altered
- **Example**
  - Chassis (vehicle) mounted antennas
- Controllable region: Ω_{c}
  - (Antenna)
  - Arbitrary configuration of vacuum & material of select properties



[Gustafsson, 2016]

Application: Embedded Design Problems

- *Embedded design:* devices containing separate regions, with only specified regions able to be altered
- **Example**
  - Chassis (vehicle) mounted antennas
- Controllable region: Ω_{c}
  - (Antenna)
  - Arbitrary configuration of vacuum & material of select properties
- Uncontrollable region: Ω_{u}
  - (Ground plane)
  - Not allowed to be altered



[Gustafsson, 2016]

Controllable / Uncontrollable Regions

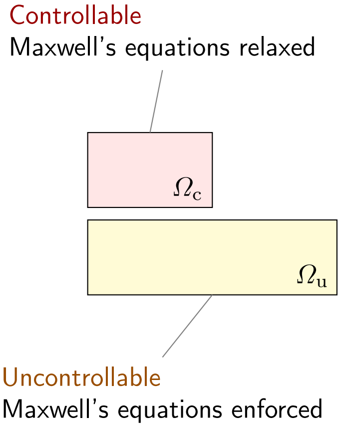
- Represent controllable / uncontrollable interaction via problem-specific Green's function

$$\begin{bmatrix} \mathbf{V}_\mathrm{u} \\ \mathbf{V}_\mathrm{c} \end{bmatrix} = \begin{bmatrix} \mathbf{Z}_\mathrm{uu} & \mathbf{Z}_\mathrm{uc} \\ \mathbf{Z}_\mathrm{cu} & \mathbf{Z}_\mathrm{cc} \end{bmatrix} \begin{bmatrix} \mathbf{I}_\mathrm{u} \\ \mathbf{I}_\mathrm{c} \end{bmatrix}$$

- Explicitly enforce Maxwell's equations on the uncontrollable region

$$\mathbf{I}_\mathrm{u} = \mathbf{Z}_\mathrm{uu}^{1} \mathbf{V}_\mathrm{u} - \mathbf{Z}_\mathrm{uu}^{1} \mathbf{Z}_\mathrm{uc} \mathbf{I}_\mathrm{c}$$

- Rewrite objectives and constraints solely in terms of controllable currents



Controllable / uncontrollable regions

Free space problem

$$
\begin{aligned}
\max_{\mathbf{I}} \quad & w_{\mathrm{a}} P_{\mathrm{a}}(\mathbf{I}) + w_{\mathrm{s}} P_{\mathrm{s}}(\mathbf{I}) \\
\text{s.t.} \quad & P_{\mathrm{a}}(\mathbf{I}) + P_{\mathrm{s}}(\mathbf{I}) = P_{\mathrm{t}}(\mathbf{I}, \mathbf{V}) \\
& W(\mathbf{I}) = W_{\mathrm{t}}(\mathbf{I}, \mathbf{V})
\end{aligned}
$$

Controllable / uncontrollable regions

Free space problem

$$
\begin{aligned}
\max_{\mathbf{I}} \quad & w_{\mathrm{a}} P_{\mathrm{a}}(\mathbf{I}) + w_{\mathrm{s}} P_{\mathrm{s}}(\mathbf{I}) \\
\text{s.t.} \quad & P_{\mathrm{a}}(\mathbf{I}) + P_{\mathrm{s}}(\mathbf{I}) = P_{\mathrm{t}}(\mathbf{I}, \mathbf{V}) \\
& W(\mathbf{I}) = W_{\mathrm{t}}(\mathbf{I}, \mathbf{V})
\end{aligned}
$$

$$A(\mathbf{I}) = \mathbf{I}^{\mathrm{H}}\mathbf{A}\mathbf{I} + \mathrm{Re}\left\{\mathbf{I}^{\mathrm{H}}\mathbf{a}\right\} + a, \quad \mathbf{I}_{\mathrm{u}} = \mathbf{C}\mathbf{V}_{\mathrm{u}} + \mathbf{D}\mathbf{I}_{\mathrm{c}}$$

$$\downarrow$$

$$\tilde{A}(\mathbf{I}_{\mathrm{c}}) = \mathbf{I}^{\mathrm{H}}\tilde{\mathbf{A}}\mathbf{I} + \mathrm{Re}\left\{\mathbf{I}^{\mathrm{H}}\tilde{\mathbf{a}}\right\} + \tilde{a}$$

Controllable / uncontrollable regions

Free space problem

$$
\begin{aligned}
\max_{\mathbf{I}} \quad & w_{\mathrm{a}} P_{\mathrm{a}}(\mathbf{I}) + w_{\mathrm{s}} P_{\mathrm{s}}(\mathbf{I}) \\
\text{s.t.} \quad & P_{\mathrm{a}}(\mathbf{I}) + P_{\mathrm{s}}(\mathbf{I}) = P_{\mathrm{t}}(\mathbf{I}, \mathbf{V}) \\
& W(\mathbf{I}) = W_{\mathrm{t}}(\mathbf{I}, \mathbf{V})
\end{aligned}
$$

Embedded problem

$$
\begin{aligned}
\max_{\mathbf{I}_{\mathrm{c}}} \quad & w_{\mathrm{a}} \tilde{P}_{\mathrm{a}}(\mathbf{I}_{\mathrm{c}}) + w_{\mathrm{s}} \tilde{P}_{\mathrm{s}}(\mathbf{I}_{\mathrm{c}}) \\
\text{s.t.} \quad & \tilde{P}_{\mathrm{a}}(\mathbf{I}_{\mathrm{c}}) + \tilde{P}_{\mathrm{s}}(\mathbf{I}_{\mathrm{c}}) = \tilde{P}_{\mathrm{t}}(\mathbf{I}_{\mathrm{c}}, \mathbf{V}) \\
& \tilde{W}(\mathbf{I}_{\mathrm{c}}) = \tilde{W}_{\mathrm{t}}(\mathbf{I}_{\mathrm{c}}, \mathbf{V})
\end{aligned}
$$

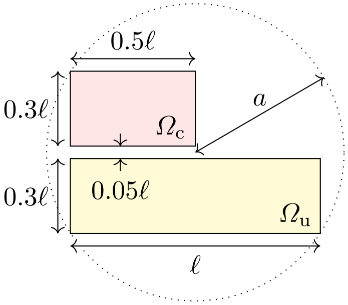
$$
A(\mathbf{I}) = \mathbf{I}^{\mathrm{H}} \mathbf{A} \mathbf{I} + \mathrm{Re}\left\{\mathbf{I}^{\mathrm{H}} \mathbf{a}\right\} + a, \quad \mathbf{I}_{\mathrm{u}} = \mathbf{C}\mathbf{V}_{\mathrm{u}} + \mathbf{D}\mathbf{I}_{\mathrm{c}}
$$

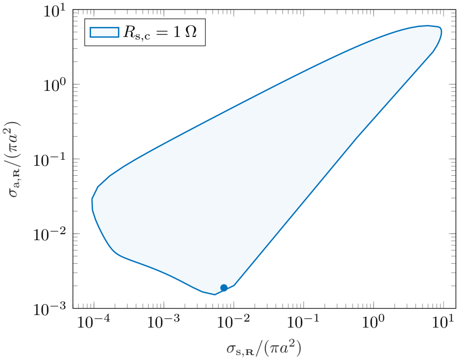
$$
\downarrow
$$

$$
\tilde{A}(\mathbf{I}_{\mathrm{c}}) = \mathbf{I}^{\mathrm{H}} \tilde{\mathbf{A}} \mathbf{I} + \mathrm{Re}\left\{\mathbf{I}^{\mathrm{H}} \tilde{\mathbf{a}}\right\} + \tilde{a}
$$

Partitioning method leads to shared structure between free space and embedded problems.

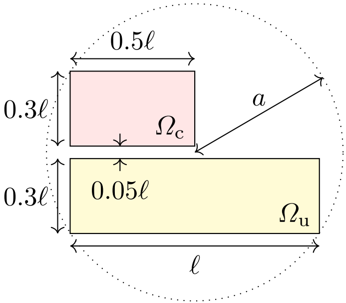
Example



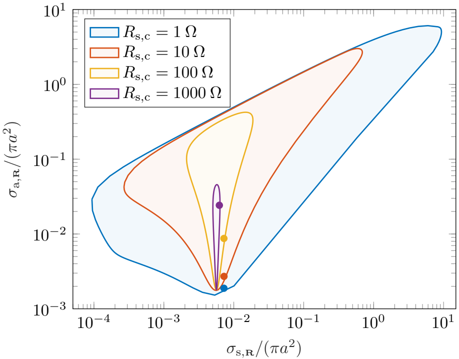


- Consider only real power conservation (allow tunable reactance, metamaterials).
- Uncontrollable region prevents perfect cloaking ($\sigma_\mathrm{a} = \sigma_\mathrm{s} = 0$).

Example

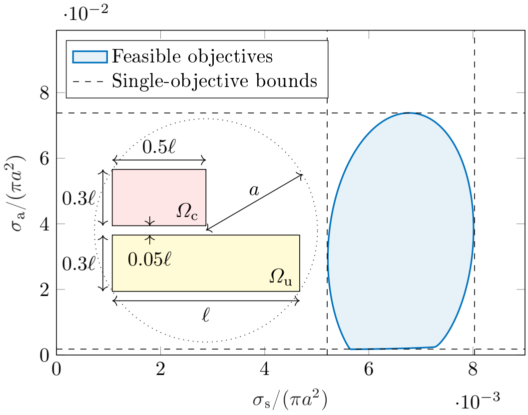


- Consider only real power conservation (allow tunable reactance, metamaterials).
- Uncontrollable region prevents perfect cloaking ($\sigma_a = \sigma_s = 0$).

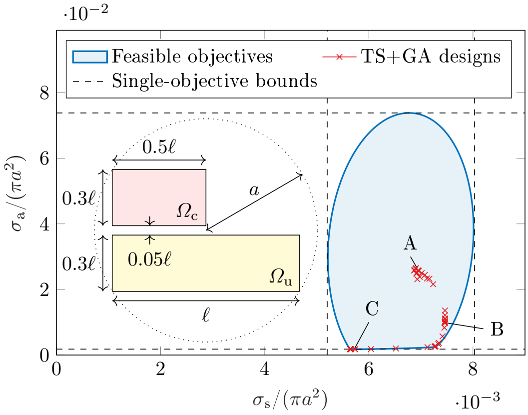


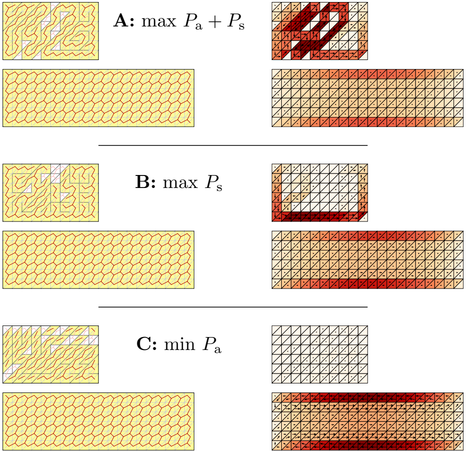
- Increased loss in controllable region restricts scattering control.

Automated Synthesis



Automated Synthesis

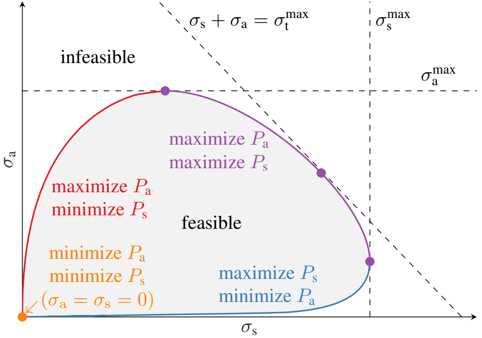




Outline

Conclusions & Future Work

- Bounds quantify *feasibility* of design objectives
- Devices with engineered behavior can be compared to their potential optimum behavior
    - ⋆ Quantify optimality of inverse design routines
- Multi-objective framework allows for multiple performance metrics to be assessed



Schab et al. "Trade-offs in absorption and scattering by nanophotonic structures," *Optics Express*, 2020.