Optimization of resonant and quasi-periodic metasurfaces

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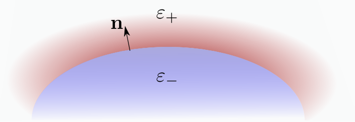
Introduction

When considering **Maxwell equations**, the tangential components of **E** and **H** are continuous across two mediums:

$$\mathbf{n} \times [\![\mathbf{E}]\!] = \mathbf{0} \quad \text{and} \quad \mathbf{n} \times [\![\mathbf{H}]\!] = \mathbf{0}.$$



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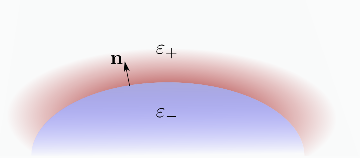

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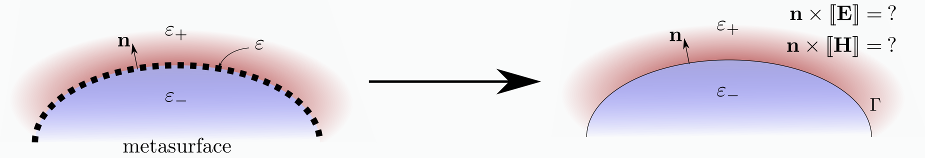
A **metasurface** is an array of **deeply subwavelength meta-atoms** with period $\delta \ll \lambda$ and thickness $\propto \delta$ (aspect ratio close to one).



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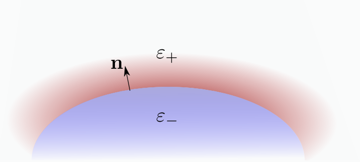

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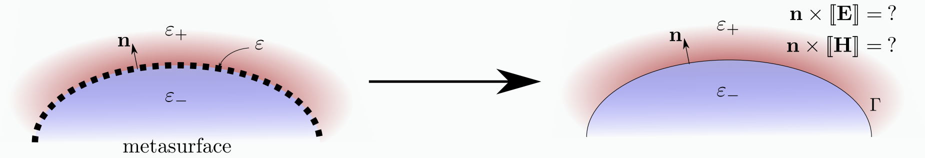


- How to find these **effective transition conditions** ?
- Can it be used to **optimize the geometry** of each meta-atom ?

Resonant meta-atoms

To obtain a non-negligible macroscopic effect of the metasurface on the incident waves, it is necessary to consider **resonant particles**.

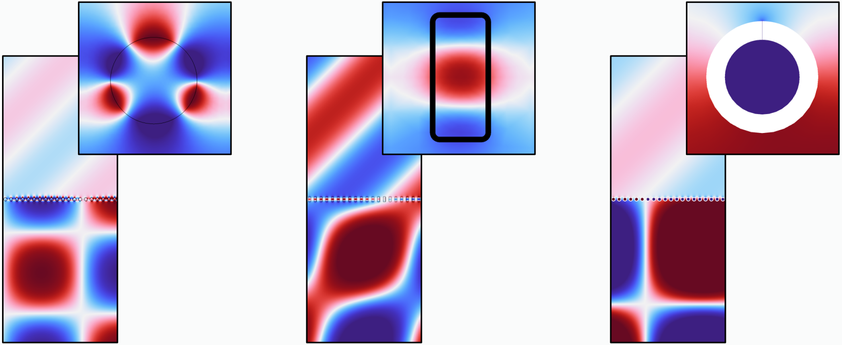
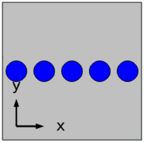


Fig. Simulations of metasurfaces with (a) Plasmonic resonances ($\varepsilon < 0$), (b) Mie resonances ($\varepsilon \gg 1$), (c) Helmholtz resonators/SSR (cavity opening $\ll \delta$).

Surface homogenization

Presentation in 2D TM only: $\mathrm{H} = \mathrm{H}_z$ solution of $\nabla \cdot \left(\frac{1}{\varepsilon_r} \nabla \mathrm{H} \right) + k_0^2 \mathrm{H} = 0$.
We consider meta-atoms made of $\varepsilon_r = \varepsilon$ and fully surrounded by air $\varepsilon_r = 1$.



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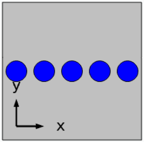
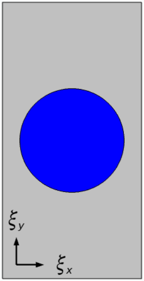
We introduce a **microscopic variable** $\boldsymbol{\xi} = \mathbf{x}/\delta$ to describe the rapid variations of the near field with $\varepsilon_r(\boldsymbol{\xi})$ and:

$$\textbf{(far field)} \quad \mathrm{H} = \sum_n \delta^n \mathrm{H}_n(\mathbf{x}),$$

$$\textbf{(near field)} \quad \mathrm{H} = \sum_n \delta^n \mathrm{h}_n(x, \boldsymbol{\xi}).$$





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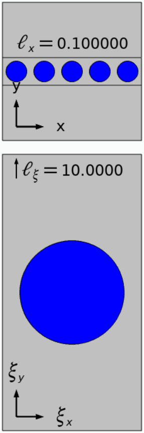


The values of the near & far fields are linked using **matching conditions** at a distance $\ell_\xi = 1/\sqrt{\delta}$:

$$\mathrm{H}_0(x, \pm 0) = \lim_{\ell_\xi \to \infty} \mathrm{h}_0(x, \xi_x, \pm \ell_\xi),$$

$$\mathrm{H}_1(x, \pm 0) = \lim_{\ell_\xi \to \infty} \mathrm{h}_1(x, \xi_x, \pm \ell_\xi) - \ell \mathrm{H}_0(x, \pm 0).$$

FAR FIELDS AT THE FIRST ORDER: GSTC

The effective field $\mathrm{H} = \mathrm{H}_0 + \delta \mathrm{H}_1$ satisfies **Generalized Sheet Transition Conditions** (GSTC):

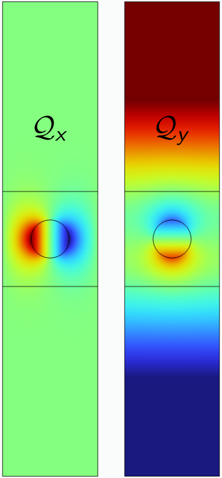
$$\llbracket \mathrm{H} \rrbracket = \chi_{ee}^{xx} \left\{ \partial_y \mathrm{H} \right\} - \chi_{ee}^{xy} \partial_x \left\{ \mathrm{H} \right\},$$
$$\llbracket \partial_y \mathrm{H} \rrbracket = \chi_{ee}^{yy} \partial_{xx} \left\{ \mathrm{H} \right\} - \chi_{ee}^{yx} \partial_x \left\{ \partial_y \mathrm{H} \right\},$$

with **surface electric susceptibility tensor** $\overline{\overline{\chi}}_{ee}$:

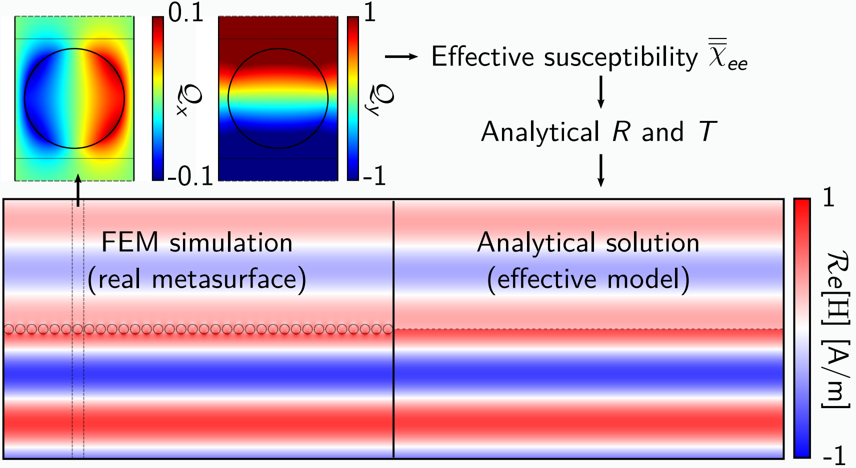
$$\overline{\overline{\chi}}_{ee} = \delta \begin{pmatrix} \llbracket \mathcal{Q}_y \rrbracket_{\xi_y = \pm\infty} & \llbracket \mathcal{Q}_x \rrbracket_{\xi_y = \pm\infty} \\ \int_Y \frac{1}{\varepsilon_r} \partial_{\xi_y} \mathcal{Q}_y \, \mathrm{d}\boldsymbol{\xi} & \int_Y 1 - \frac{1}{\varepsilon_r} \partial_{\xi_x} \mathcal{Q}_x \, \mathrm{d}\boldsymbol{\xi} \end{pmatrix},$$

and **elementary problems** $\mathcal{Q}_\iota$, $\iota = x, y$ given by:

$$\begin{cases} \nabla_{\boldsymbol{\xi}} \cdot \left(\frac{1}{\varepsilon_r} \left(\mathbf{u}_\iota + \nabla_{\boldsymbol{\xi}} \mathcal{Q}_\iota \right) \right) & = 0 \\ \lim_{\xi_y \to \infty} \partial_{\xi_y} \mathcal{Q}_\iota & = 0 \end{cases}.$$



To summarize ...



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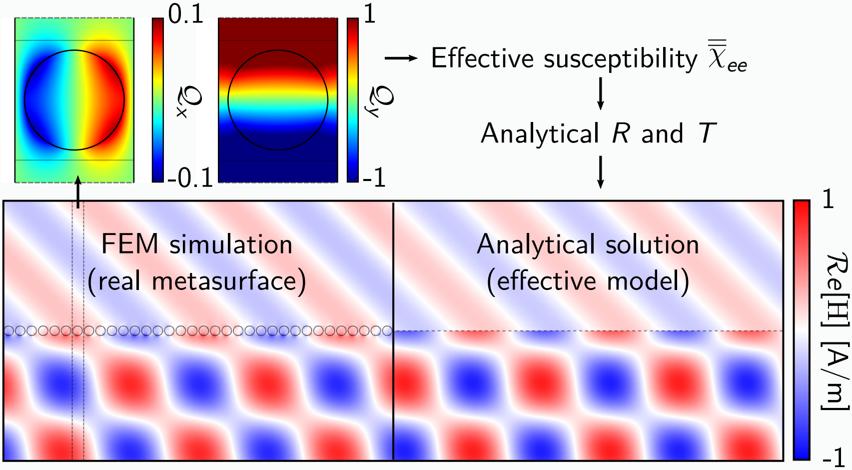

Localized surface plasmon

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There exists **plasmonic modes** $(\varepsilon_n, \mathcal{Q}_n)$ with $\varepsilon_n < 0$ solutions to:

$$\begin{cases} \nabla \cdot \left(\frac{1}{\varepsilon_n} \nabla \mathcal{Q}_n\right) = 0 & \text{inside} \\ \Delta \mathcal{Q}_n = 0 & \text{outside} \end{cases} \quad \Rightarrow \quad \text{for } \textbf{any } \varepsilon,\ \iota = x, y;\ \mathcal{Q}_\iota = \sum_n \alpha_n^\iota \mathcal{Q}_n.$$

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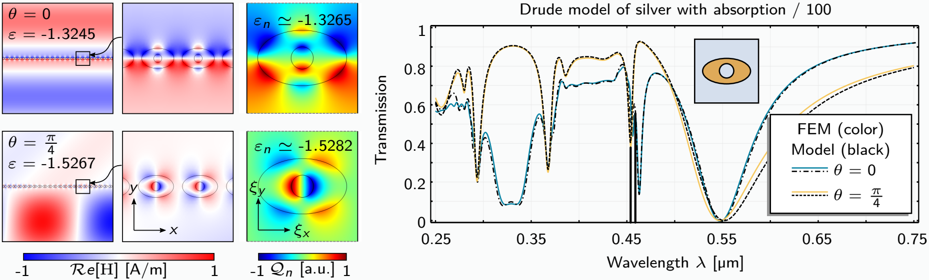
When ε is given by a dispersive relation $\varepsilon(\lambda)$, its spectrum crosses the ε_n:



Finite element implementation

When not periodic, we need **simulations of the full metasurface**.

If $\varepsilon(x, \boldsymbol{\xi})$ (locally-periodic microscopically) then:

$$
\begin{aligned}
[\![\mathrm{H}]\!] &= \chi_{ee}^{xx}(x)\{\partial_y \mathrm{H}\} - \chi_{ee}^{xy}(x)\partial_x \{\mathrm{H}\}, \\
[\![\partial_y \mathrm{H}]\!] &= \partial_x \left(\chi_{ee}^{yy}(x)\partial_x \{\mathrm{H}\}\right) - \partial_x \left(\chi_{ee}^{yx}(x)\{\partial_y \mathrm{H}\}\right).
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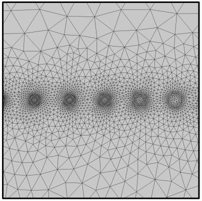
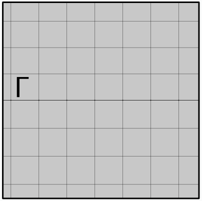


The **variational formulation** of H is given by:

$$\int_{\mathcal{D}} \nabla \mathrm{H} \cdot \nabla \phi^* - k_0^2 \mathrm{H}\phi^* \, \mathbf{dx} + \int_\Gamma \underbrace{[\![\partial_y \mathrm{H}\phi^*]\!]}_{[\![\partial_y \mathrm{H}]\!]\{\phi^*\}+\{\partial_y \mathrm{H}\}[\![\phi^*]\!]} \mathrm{d}x = 0,$$

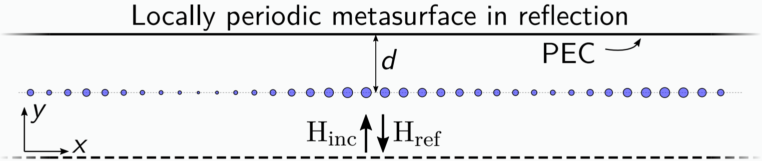
where in particular:

$$\int_\Gamma [\![\partial_y \mathrm{H}]\!] \{\phi^*\} \mathrm{d}x = \int_\Gamma (\chi_{ee}^{yx}\{\partial_y \mathrm{H}\} - \chi_{ee}^{yy}\partial_x \{\mathrm{H}\})\partial_x\{\phi^*\} \mathrm{d}x.$$



Metasurfaces in reflection

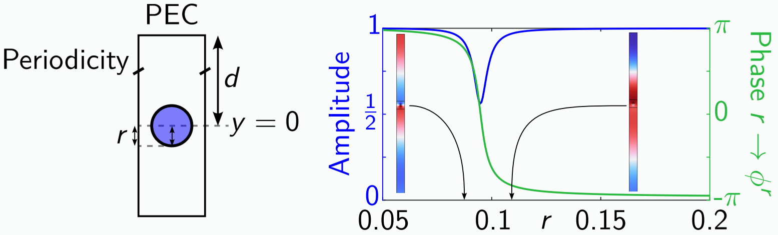
In the next examples, we will consider a metasurface placed at a distance d from a perfect reflector.

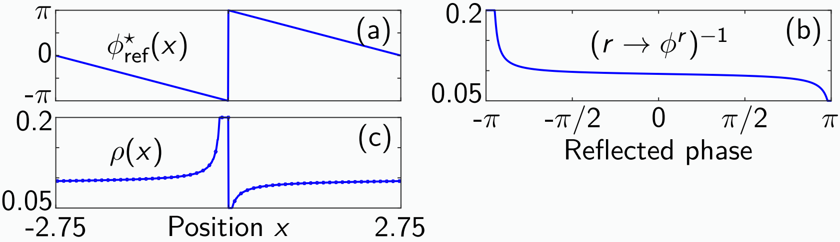


For a normal-incident plane wave $\mathrm{H}_{\mathrm{inc}}$, we want to **find the distribution of radius** ρ such that the reflected field $\mathrm{H}_{\mathrm{ref}}$ is as close as possible to a target $\mathrm{H}^{\star}_{\mathrm{ref}}$.

Design with local phase changes 1/2

Classicaly, the design of a metasurface is obtained using the local phase induced by meta-atoms if they were placed in a periodic environment.





Design with local phase changes 2/2

To obtain a deflector with $\mathrm{H}_{\mathrm{inc}} = e^{-ik_0 y}$ and $\mathrm{H}_{\mathrm{ref}} = e^{-ik_0(\sin(\theta)x - \cos(\theta)y)}$, the phase change on Γ must follow (Generalized Snell law):

$$\phi(x) = k_0 \sin(\theta) x.$$

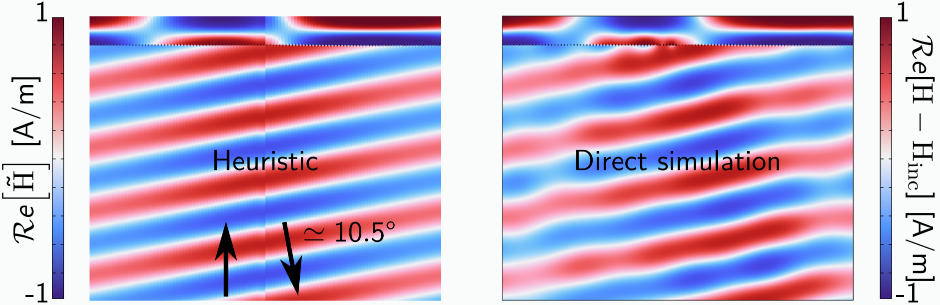


Fig. (left) Design of a metasurface using local phases. (right) FEM simulation.

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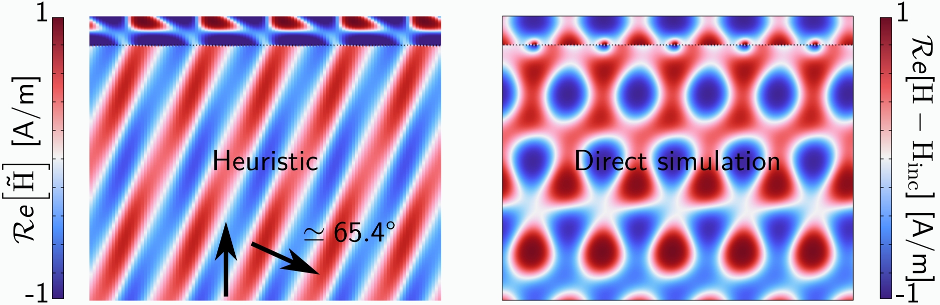

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Gradient-based optimization

Instead of a parametric optimization (radius of each meta-atom), we have to find a distribution $\rho^* : \Gamma \to (r_{\min}, r_{\max})$ **maximizing a functional** $F(\rho)$:

$$\rho^* := \arg\max_{\rho} F(\rho),$$

solved using a **gradient-based algorithm** based on the Taylor expansion:

$$F(\rho_n + \epsilon\tilde{\rho}) = F(\rho_n) + \epsilon \int_\Gamma G(\rho_n)\tilde{\rho}\,\mathrm{d}x + o(\epsilon) \quad \text{s.t.} \quad F(\underbrace{\rho_n + \epsilon G(\rho_n)}_{\rho_{n+1}}) > F(\rho_n).$$

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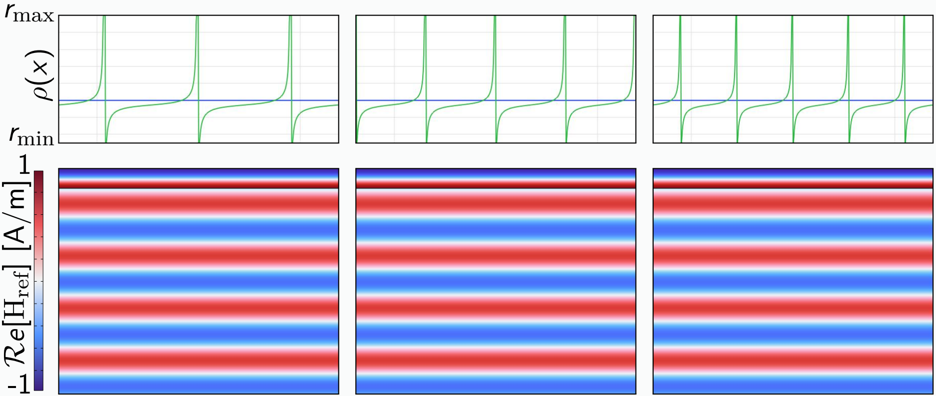
- Numerically, $G(\rho_n)$ is obtained via the solution of an **adjoint state**.

- The distribution ρ is discretized on Γ with P1 elements. To **keep the quasi-periodicity**, we use a **regularized** version $K(\rho)$ solution to:

$$-\nu\partial_{xx}K(\rho) + K(\rho) = \rho \quad \text{with a small value } \nu > 0.$$

Application: Deflectors

Optimization of deflectors for different reflection angles.



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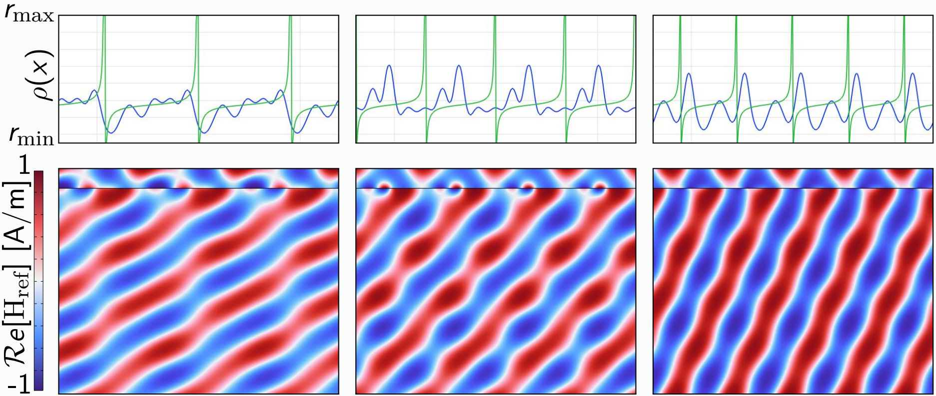

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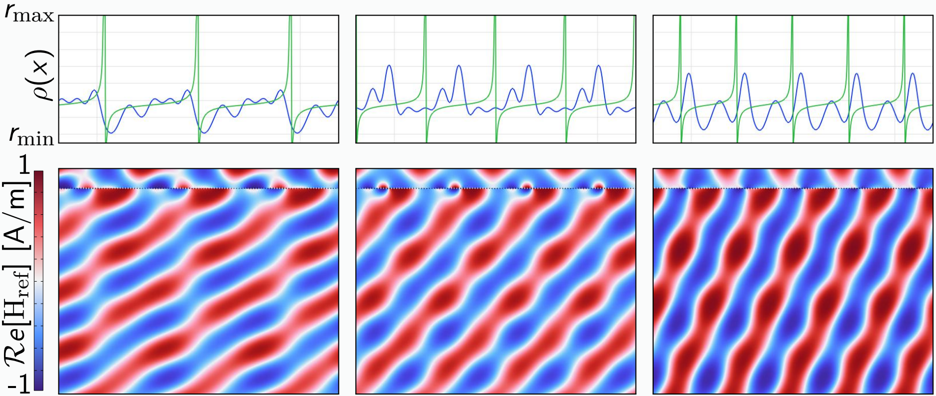
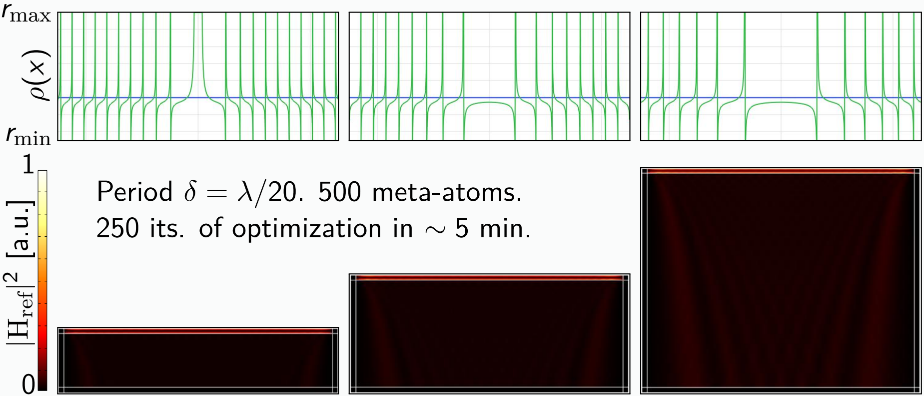


N	-1	-2	-3	-4	-5
Local method	76 %	71 %	59 %	59 %	49 %
Optimized	79 %	80 %	82 %	80 %	78 %

APPLICATION: LENSES 1/2

Second example: **metalenses** working in reflection.

We consider a finite-size metasurface and we want to maximize the reflected energy at the focal point $\mathbf{f}_0 = (0, f_0)$, i.e. $F(\rho) = |\mathrm{H}(\mathbf{f}_0) - e^{ikf_0}|^2$.



Period $\delta = \lambda/20$. 500 meta-atoms.
250 its. of optimization in ~ 5 min.

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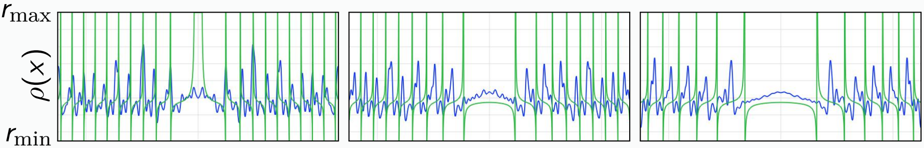

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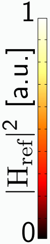

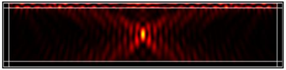

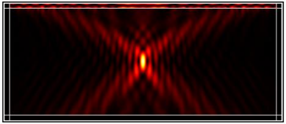

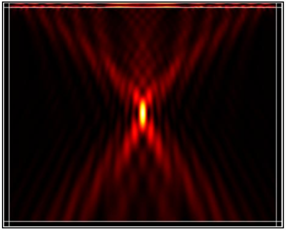

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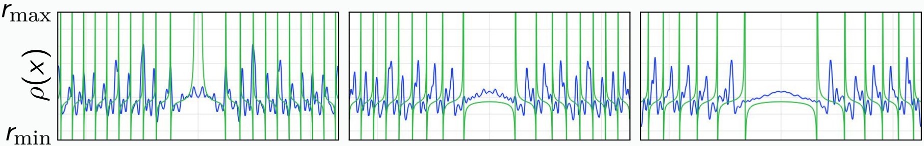

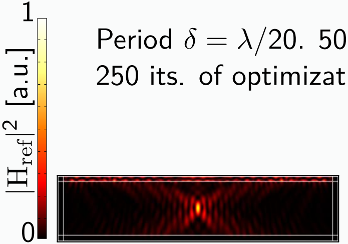

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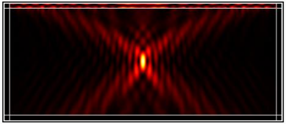
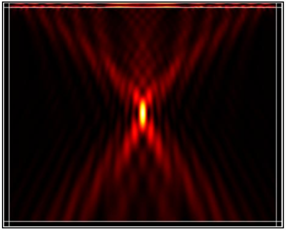
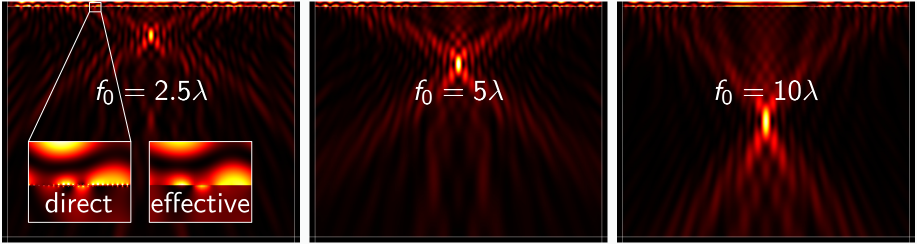




Application: Lenses 2/2

Direct simulations of the resulting designs:



The **focusing efficiencies** (percentage of the incident power reflected “near” the focal point) are given by:

f_0/λ_0	5	10	15	20
Local method	23 %	34 %	38 %	42 %
Optimized	38 %	51 %	53 %	53 %

Conclusion

- **Surface homogenization** can be used to obtain **effective transition conditions** which describes **quasi-periodic metasurfaces**. The model is even valid in the presence of **plasmonic resonances**.
- The **fast simulations** of the effective model can be used to **optimize** the performances of resonant metasurfaces.

N. Lebbe, K. Pham and A. Maurel "*Homogenized transition conditions for plasmonic metasurfaces based on quasi-static eigenmode expansion*" Physical Review B, vol. 107, no 8 (2023)

N. Lebbe, K. Pham and A. Maurel "*Optimization of plasmonic metasurfaces using quasi-periodic surface homogenization*" in preparation

→ Other resonances (Mie, SRR), 3D (already done without resonances) ...