A Nonlocal-Gradient Descent Method for Inverse Design in Nanophotonics

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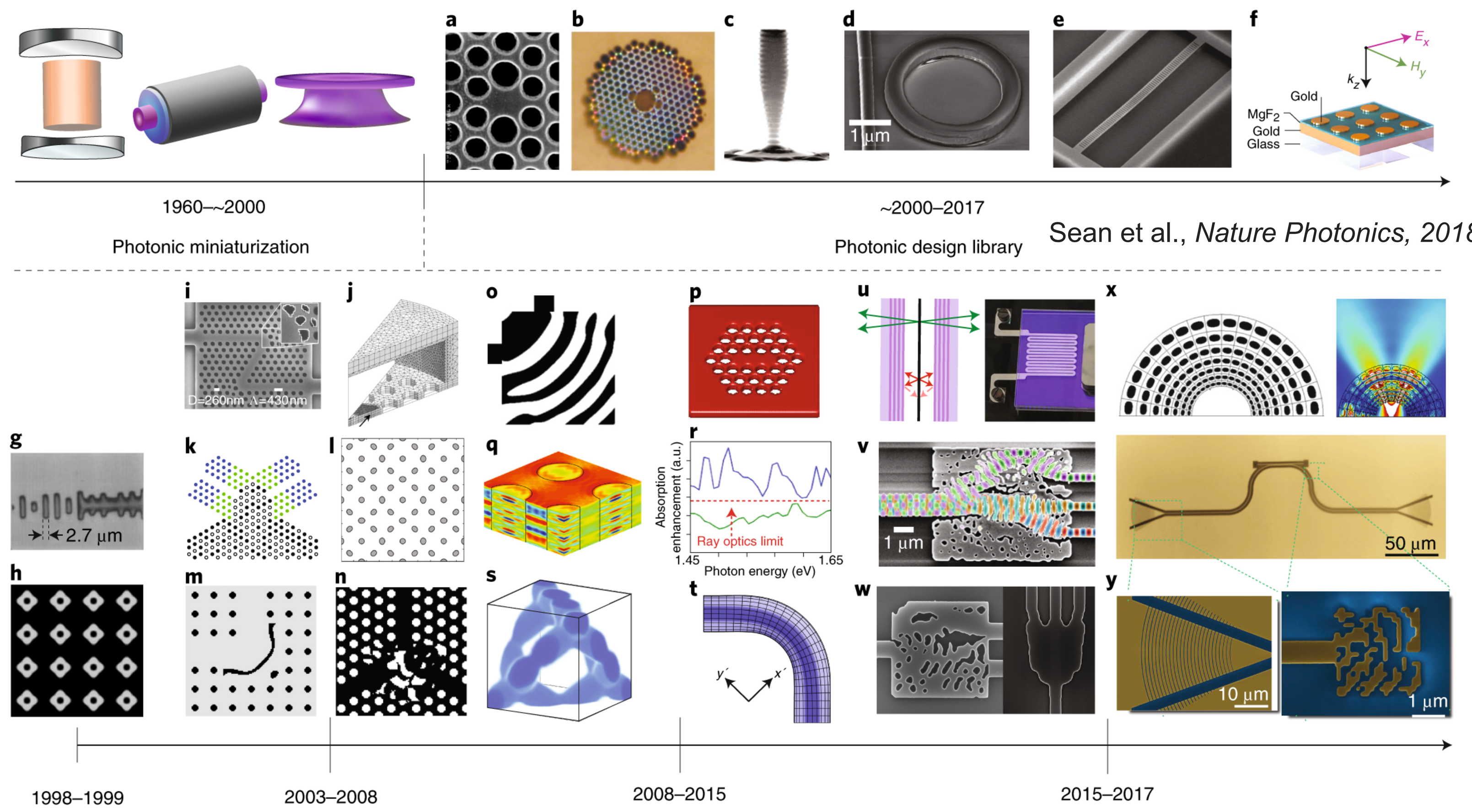
Nanophotonic devices

Computational Inverse design approaches for discovering optical structures based on desired functional characteristics. Key progress in this emerging field of photonic device optimization and design



Sean et al., *Nature Photonics*, 2018

Grand challenges in computational inverse design

- Gradient-based methods need several assumptions, e.g., statics, linear, homogeneous, and isotropic materials and time-harmonic behavior
- Gradient relies on the adjoint method may be not accessible and reliable
- Local gradient methods often converges to a local minimum
- Gradient-free methods have limitations to scale to high dimensions
- Constrained optimization (SGD, Adam, etc., did not work)

Mathematical formulation of inverse design

Generic electromagnetic design problem

$$\min_{\mathbf{x}} \; f(\mathbf{E}_1,\dots,\mathbf{E}_n,\epsilon_1,\dots,\epsilon_n,\mathbf{x})$$
$$\text{subject to} \quad g_j(\mathbf{x}) = 0, \quad j=1,\dots,m$$
$$h_k(\mathbf{x}) \le 0, \quad j=1,\dots,l$$

Maxwell's equations

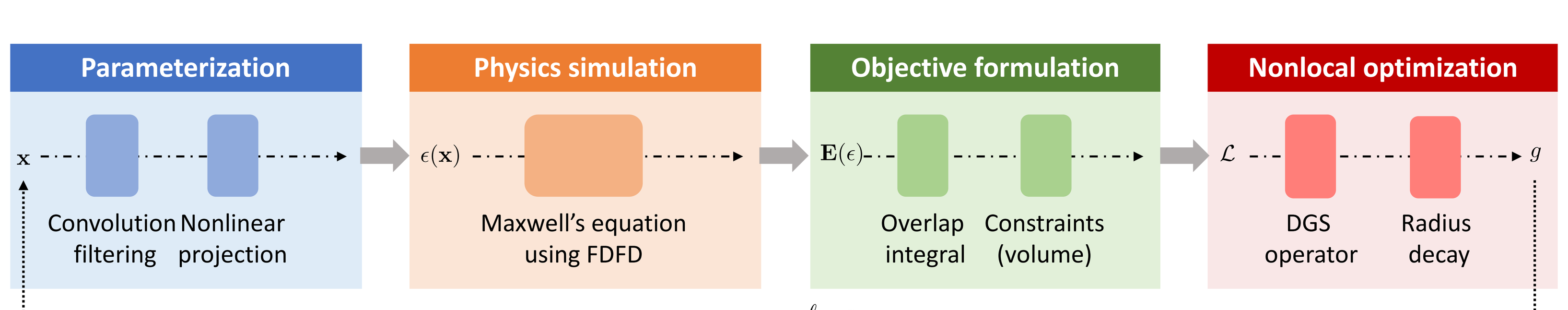
$$\nabla \times \frac{1}{\mu}\nabla \times \mathbf{E}_1 - \omega_1^2 \epsilon(\mathbf{x})\mathbf{E}_1 = -i\omega_1 \mathbf{J}_1$$
$$\nabla \times \frac{1}{\mu}\nabla \times \mathbf{E}_2 - \omega_2^2 \epsilon(\mathbf{x})\mathbf{E}_2 = -i\omega_2 \mathbf{J}_2$$

A typical objective is to maximize the transmission $f_{obj}(\mathbf{x}) = -|\mathbf{c}^\dagger \mathbf{E}(\epsilon(\mathbf{x}))|^2$

Parameterization and constraints $\epsilon(\mathbf{x}) = \epsilon_b(\mathbf{x}) + \mathbb{H}(\varphi(\mathbf{x}))$ $\;h_1(\mathbf{x}) = V(\mathbf{x})/V_0 \le \gamma$

Gradient-based optimization via derivative analysis

$$\frac{df_{obj}}{d\mathbf{x}} = \frac{\partial f_{obj}}{\partial \mathbf{x}} + 2\mathscr{R}\left[\sum_i \left(\frac{\partial f_{obj}}{\partial \mathbf{E}_i}\frac{d\mathbf{E}_i}{dx} + \frac{\partial f_{obj}}{\partial \epsilon_i}\frac{d\epsilon_i}{dx}\right)\right]$$



Directional Gaussian smoothing method

Key idea:

- average objective function along d orthogonal directions for the partial derivatives,
- assemble all partial derivatives to obtain the full search direction.

Define a *one-dimensional* function

$$G(y\,|\,\boldsymbol{x},\boldsymbol{\xi}) = F(\boldsymbol{x} + y\boldsymbol{\xi}), \quad y \in \mathbb{R}.$$

Define the Gaussian smoothing of $G(y)$, denoted by $G_\sigma(y)$, by

$$G_\sigma(y\,|\,\boldsymbol{x},\boldsymbol{\xi}) := \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} G(y+\sigma v\,|\,\boldsymbol{x},\boldsymbol{\xi})\, e^{-\frac{v^2}{2}}\, dv$$
$$= \mathbb{E}_{v\sim\mathcal{N}(0,1)}\left[G(y+\sigma v\,|\,\boldsymbol{x},\boldsymbol{\xi})\right].$$

The derivative of $G_\sigma(y|\boldsymbol{x},\boldsymbol{\xi})$ at $y=0$ is represented by

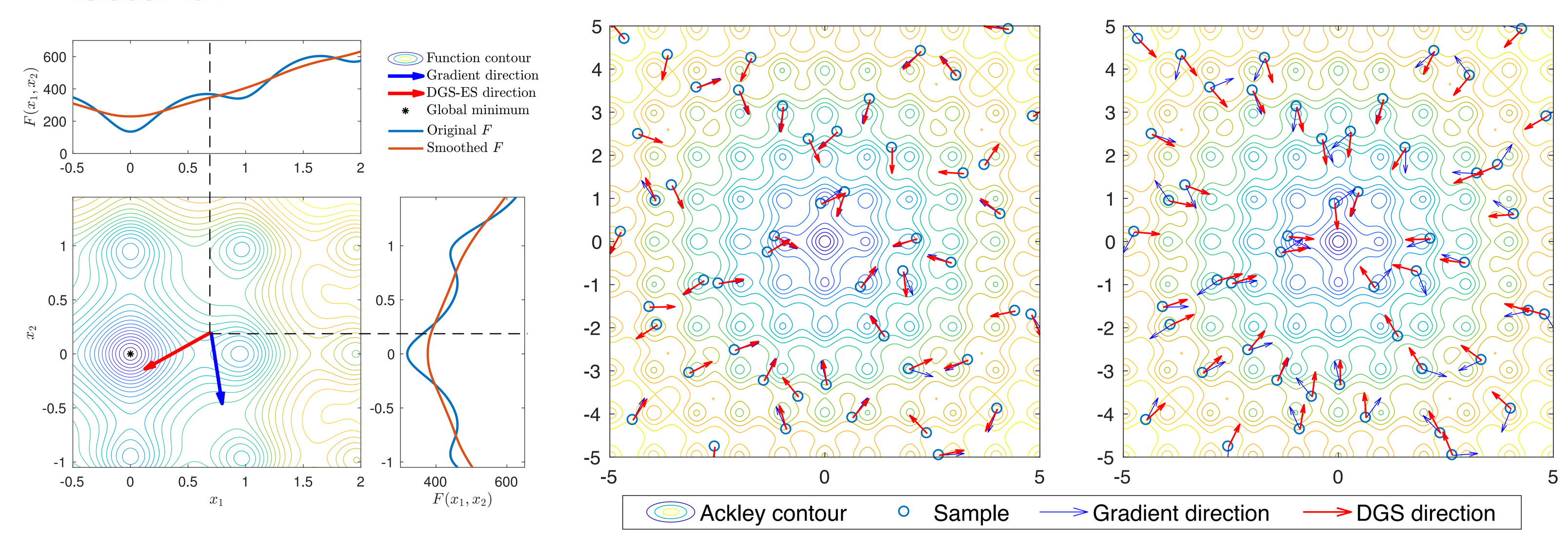
$$\mathscr{D}[G_\sigma(0\,|\,\boldsymbol{x},\boldsymbol{\xi})] = \frac{1}{\sqrt{2\pi}\sigma}\int_{\mathbb{R}} G(\sigma v\,|\,\boldsymbol{x},\boldsymbol{\xi})\, v\, e^{-\frac{v^2}{2}}\, dv,$$
$$= \frac{1}{\sigma}\mathbb{E}_{v\sim\mathcal{N}(0,1)}\left[G(\sigma v\,|\,\boldsymbol{x},\boldsymbol{\xi})\, v\right],$$

where $\mathscr{D}$ denotes the differential operator.

- Let $\Xi := (\boldsymbol{\xi}_1,\dots,\boldsymbol{\xi}_d)^\top$ represent the matrix consisting of d orthonormal vectors.
- Define a DGS-gradient operator

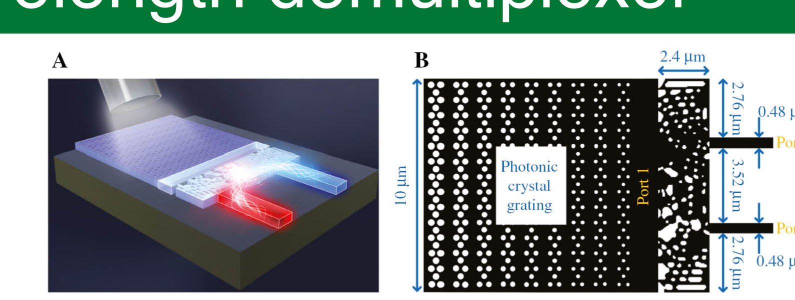
$$\nabla_{\sigma,\Xi}[F](\boldsymbol{x}) = \Xi^\top \begin{bmatrix} \mathscr{D}\left[G_{\sigma_1}(0\,|\,\boldsymbol{x},\boldsymbol{\xi}_1)\right] \\ \vdots \\ \mathscr{D}\left[G_{\sigma_d}(0\,|\,\boldsymbol{x},\boldsymbol{\xi}_d)\right] \end{bmatrix}.$$

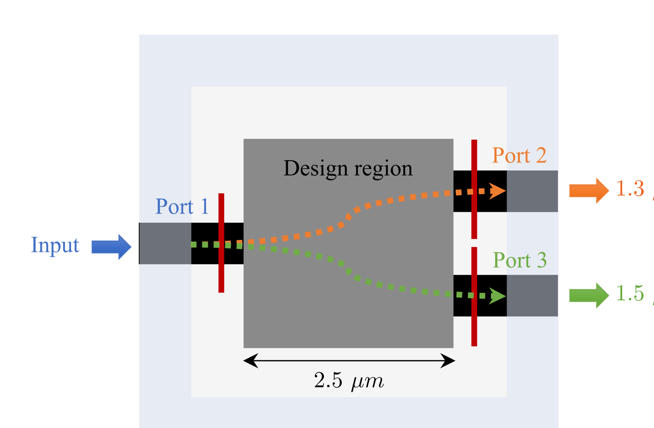
- DGS-gradient depends on Ξ and is different from $\nabla F_\sigma(\boldsymbol{x})$ for a general smoothing factor $\boldsymbol{\sigma}$.



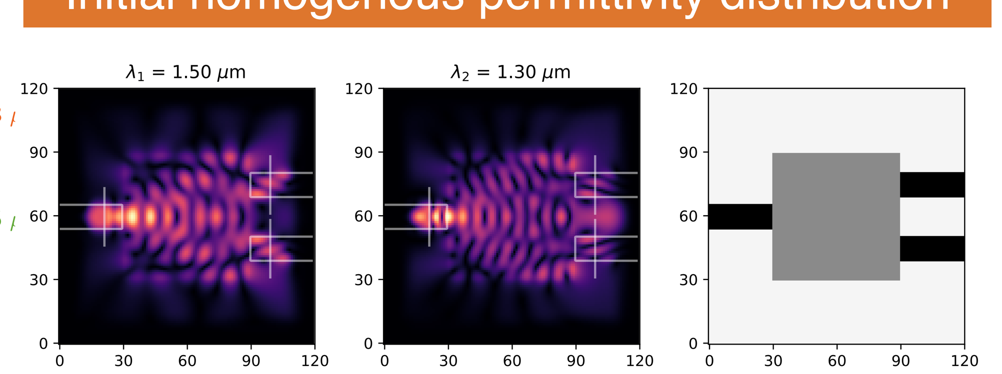
Inverse design of wavelength demultiplexer

Wavelength demultiplexer is the key components of photonic integrated circuits (PIC)

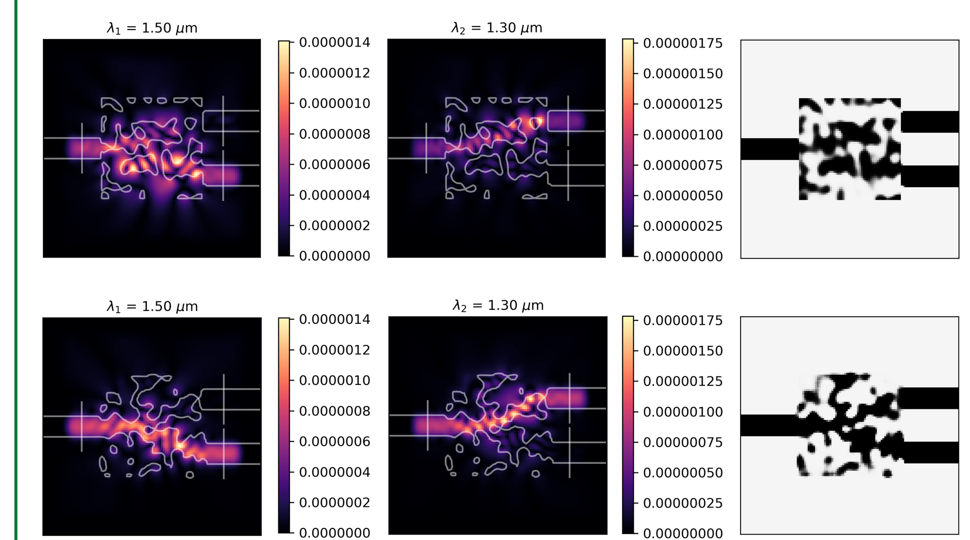




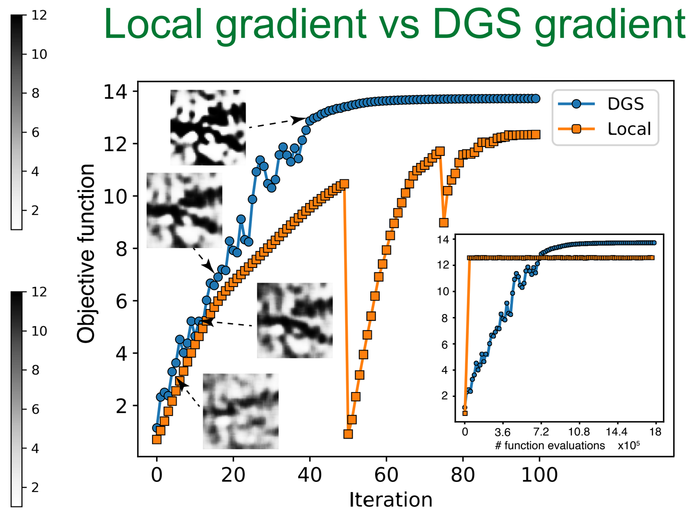
Initial homogenous permittivity distribution



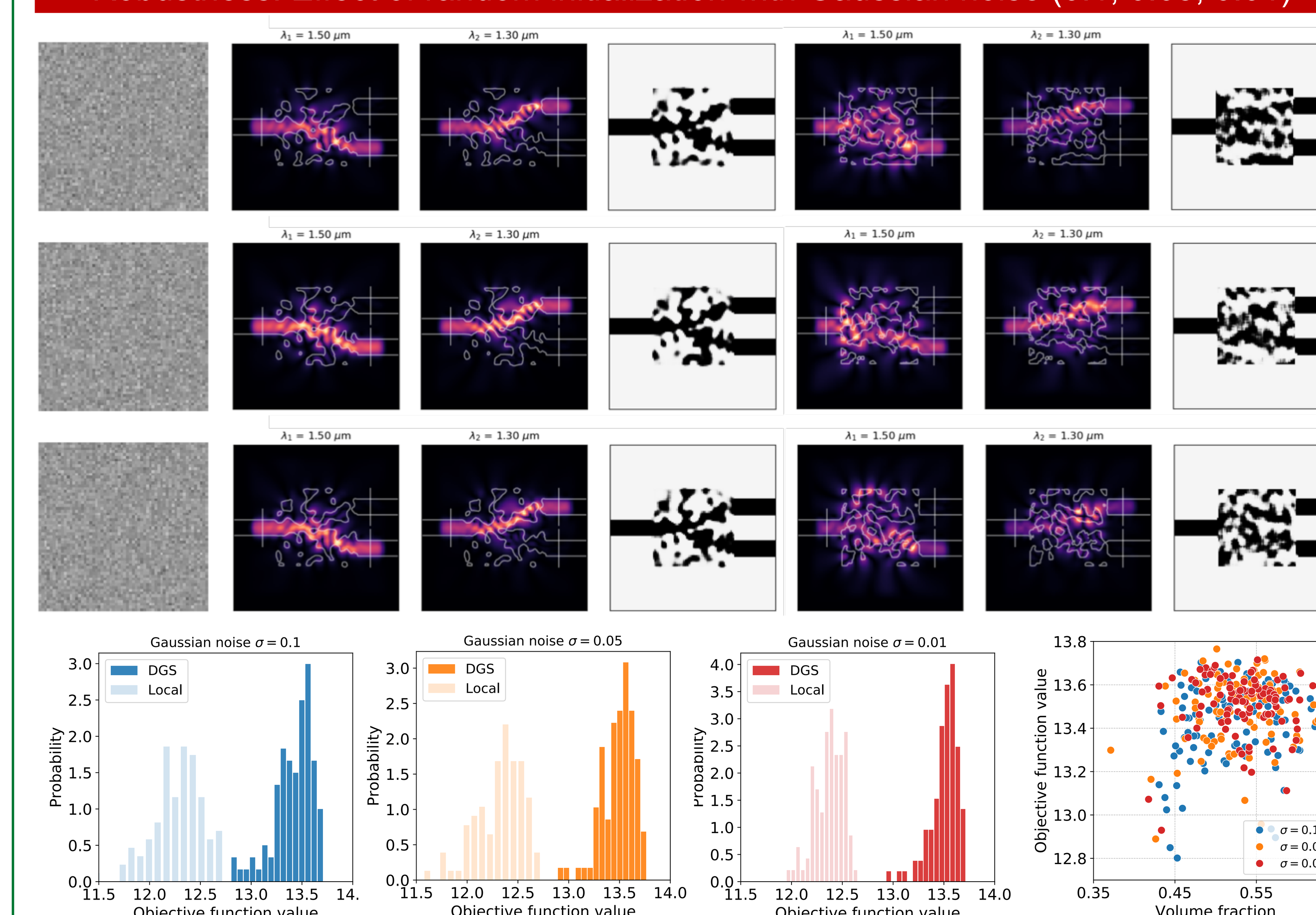
Results and discussion



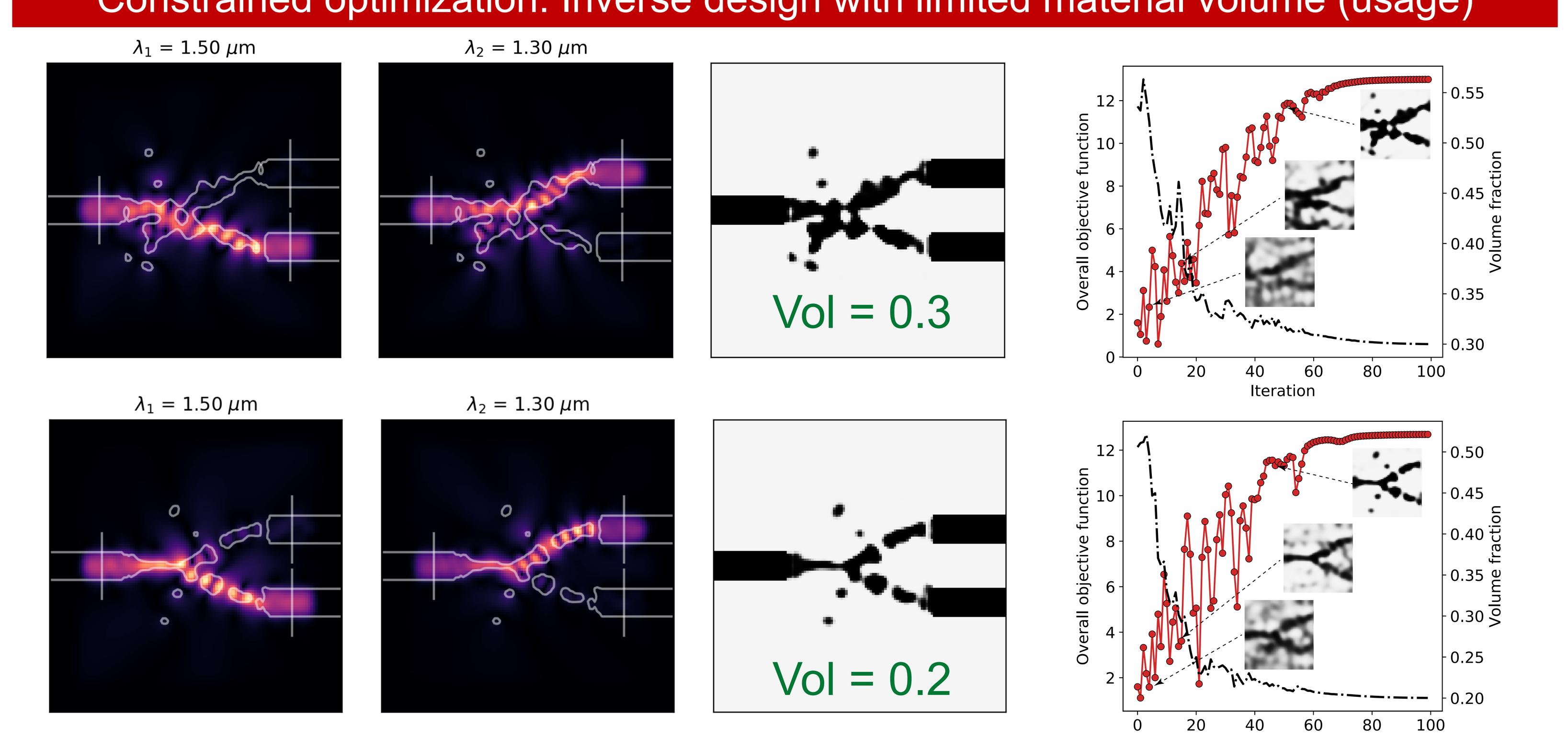
Local gradient vs DGS gradient



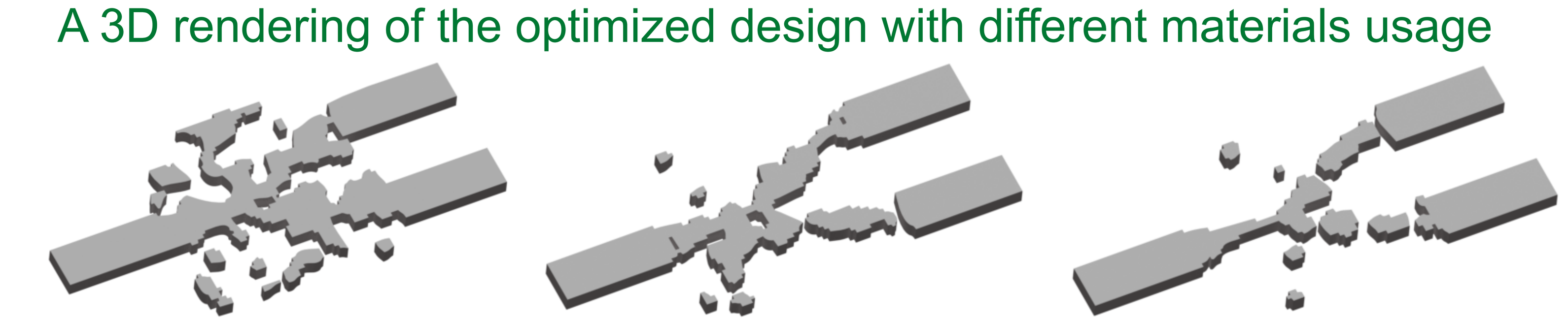
Robustness: Effect of random initialization with Gaussian noise (0.1, 0.05, 0.01)



Constrained optimization: Inverse design with limited material volume (usage)



A 3D rendering of the optimized design with different materials usage



Vol = 0.474 Vol = 0.3 Vol = 0.2