Physics-guided Diffusion Models for Inverse Design

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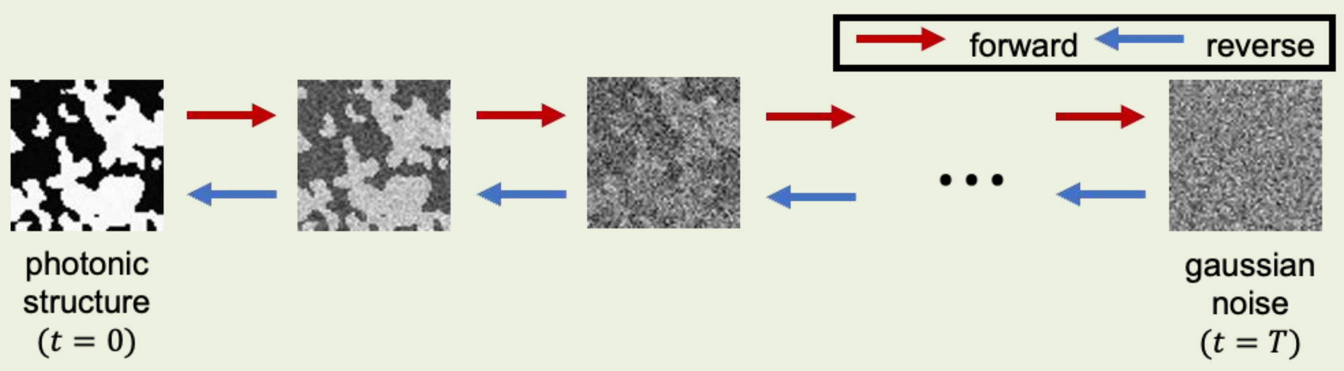
1. Motivation

- The adjoint method is effective in optimizing photonic structures by calculating the physical gradient of the entire structure with only two simulations.
- Despite its usefulness, the method often encounters limitations, including **susceptibility to local optima** and a **complicated binarization process**.
- **Deep-learning-based approaches such as GANs** formulate inverse design problems as image generation task to solve the issue but **require a large number of simulations**.
- By **combining diffusion models with adjoint sensitivity analysis**, we demonstrate that stochastic optimization with a simple process can solve an inverse problem using a minimal number of simulations.

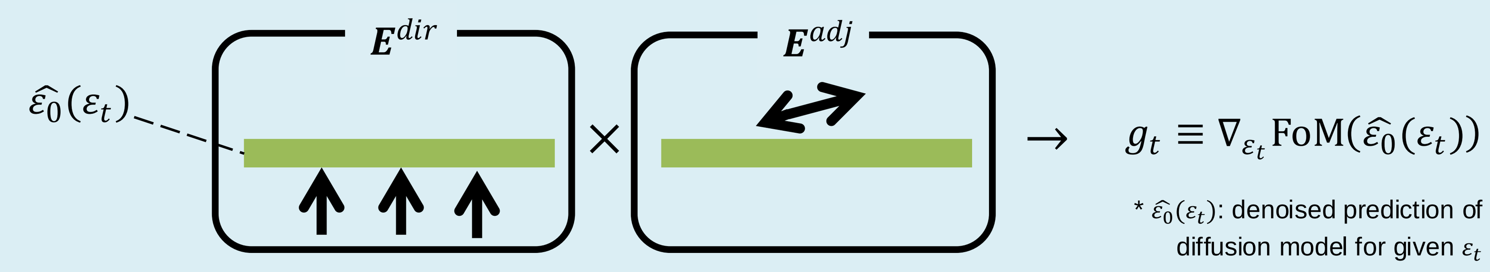
2. Methods

Diffusion Models



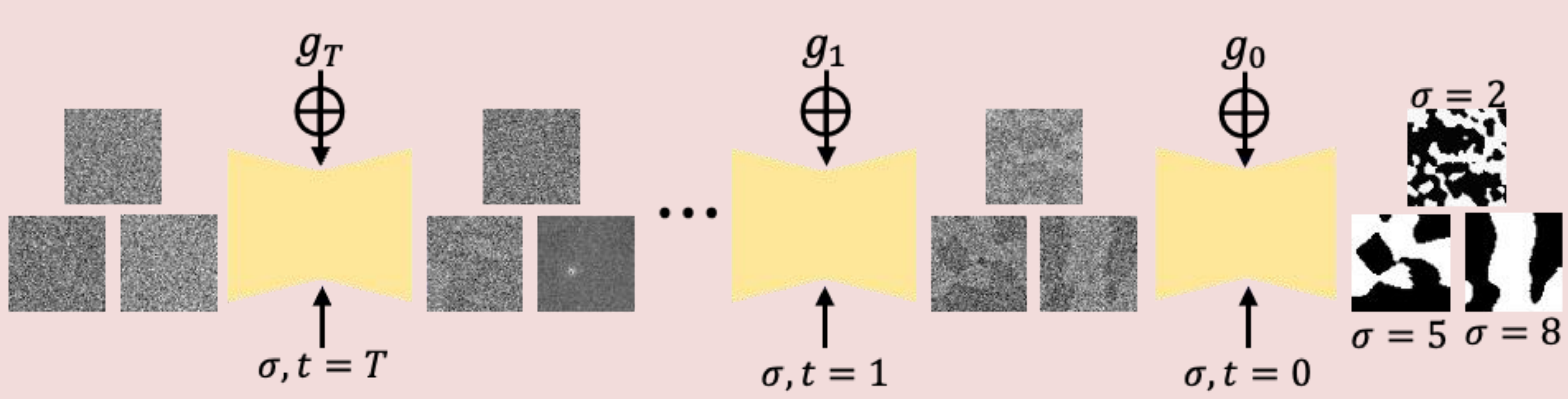
- We utilize Denoising Diffusion Probabilistic Models (DDPM).
  1) Forward process: addition of noise
  2) Reverse process: denoising process / image generation
- We apply physical gradient (adjoint gradient) to the reverse process.

Adjoint Sensitivity Analysis



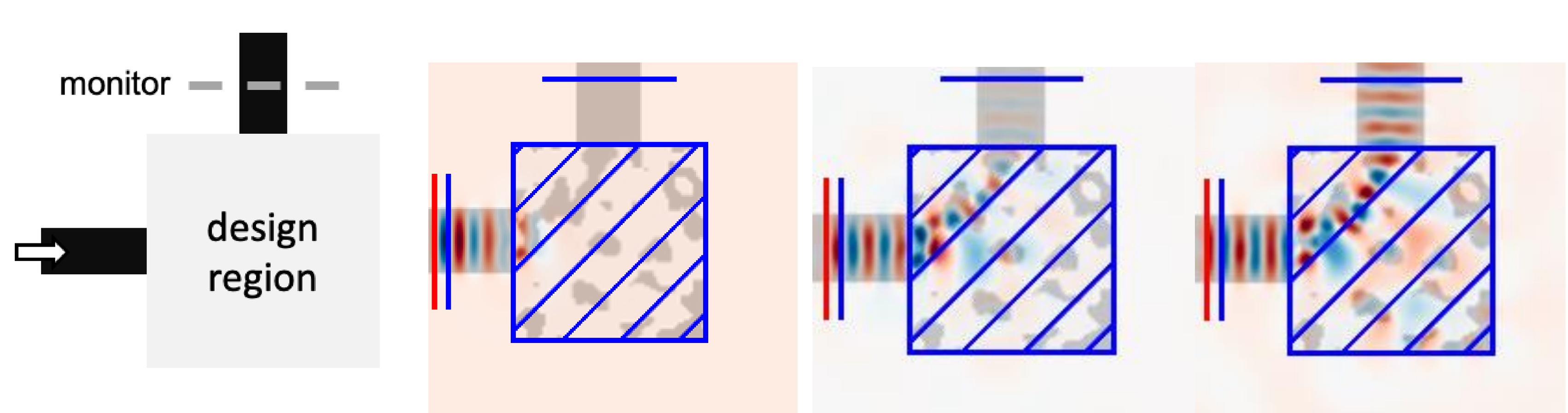
- Adjoint sensitivity analysis enables the calculation of adjoint gradient for each material pixel with only two simulations.
- Adjoint gradient indicates how the material value must change to enhance the Figure of Merit (FoM).

$$\varepsilon_{t-1} = \boldsymbol{\mu}_{\boldsymbol{\theta}}(\varepsilon_t, t) + \boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{1/2}(\varepsilon_t, t)\, \boldsymbol{z} + \eta \nabla_{\varepsilon_t} \mathrm{FoM}\left(\hat{\varepsilon}_0(\varepsilon_t)\right), \quad \boldsymbol{z} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

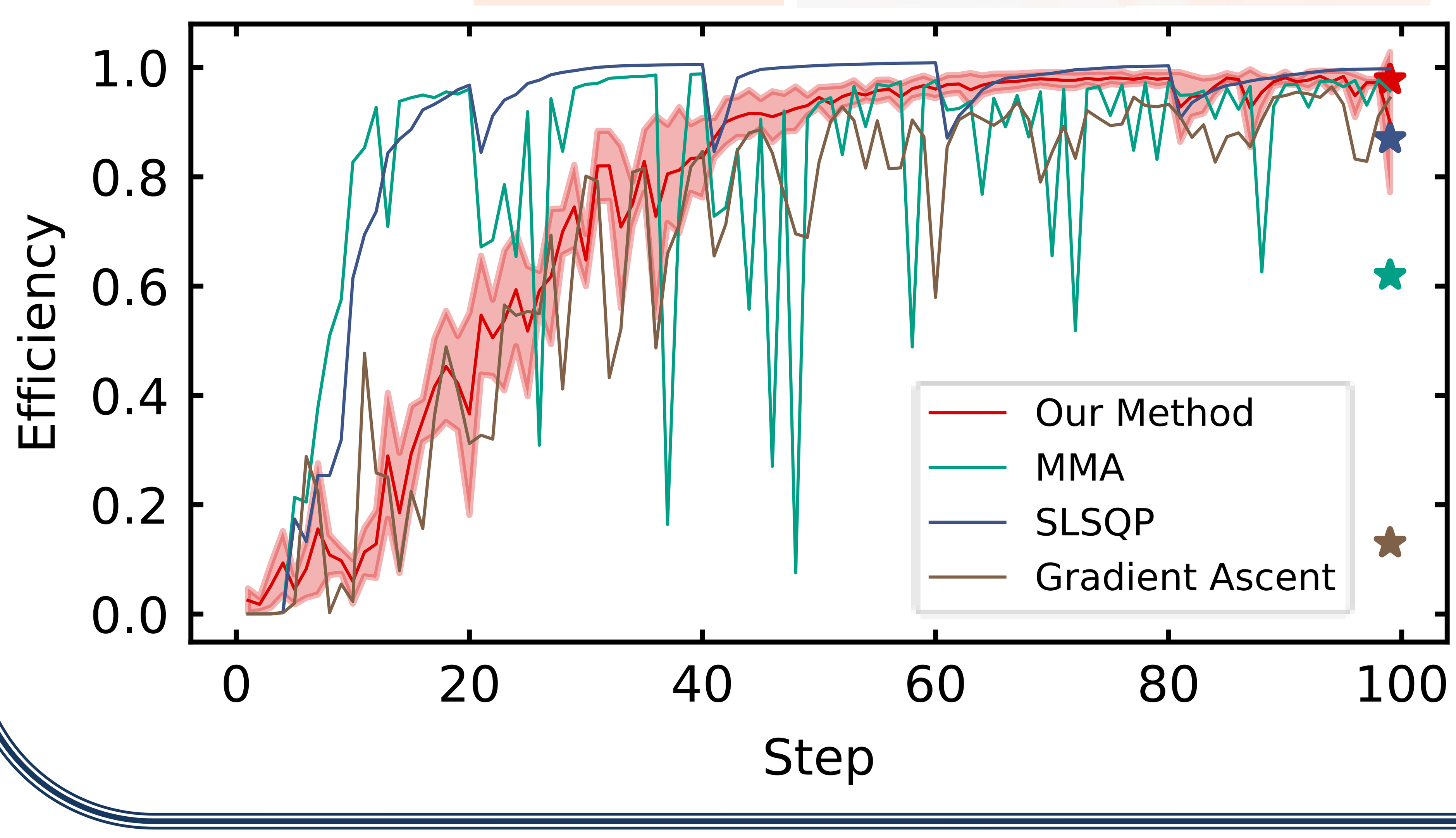


- The gradient value is directly added with the conditions of structure and the corresponding step number.
- The overall number of simulations required is determined solely by the number of reverse steps needed.

3. Results & Analysis



Problem Setup: Free-form Bending Waveguide



- The efficiency of generated structure at each step is plotted.

(efficiency of structures **after binarization** is marked with an **asterisk**)

- Despite inherent randomness (shaded region representing standard deviation), our method consistently designs high-performance devices and outperforms other algorithms.
- **MMA (Method of Moving Asymptotes)** and **SLSQP(Sequential Least Squares Quadratic Programming)** are the state-of-the-art nonlinear algorithms for adjoint optimization.