Datasets and Benchmarks for Nanophotonic Structure and Parametric Design Simulations

Joint work with Mingxuan Li, Oliver Hinder, and Paul W. Leu

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Motivation

- Nanophotonic structures play a crucial role for a wide range of real-world applications such as solar cells, anti-reflective coatings, electromagnetic interference shielding, optical filters, and light emitting diodes.
- Electrodynamic simulations, based on Maxwell's equations, provide accurate predictions of the optical and electromagnetic properties of such nanophotonic structures.
- These simulations enable us to model electromagnetic fields over time and calculate optical properties.
- Leveraging the utility of these simulations, we can combine them with optimization procedures to design and discover new and improved structures.

Contributions

- Development of a generic simulation scheme and pipeline for nanophotonic structures in Python, based on the open-source software, Meep, and licensed under the MIT license.
- Creation of datasets of a myriad of nanophotonic structures for electromagnetic interference shielding, anti-reflection, and solar cells.
- Investigation into the effects of altering grid sizes in electrodynamic simulations, providing insights into tradeoffs between computational time and simulation accuracy.
- Introduction of benchmarks specifically designed for the optimization of parametric structures, facilitating the evaluation and comparison of different optimization algorithms.

Electrodynamic Simulations

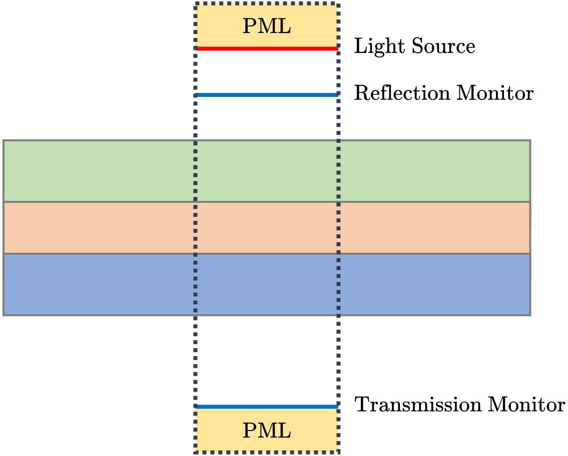
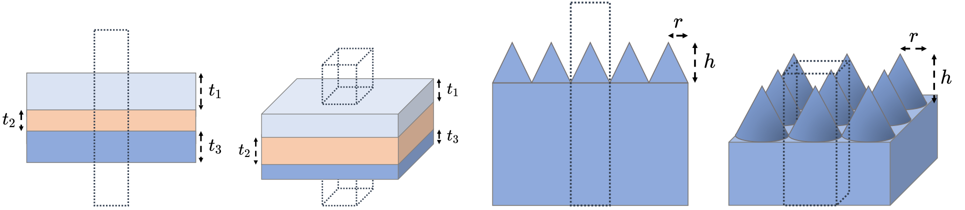


Figure 1: Schematic of nanophotonic structure simulations. Perfectly matched layers, light source, and reflection and transmission monitors are located in a simulation cell indicated by the dotted rectangle.

Nanophotonic Structures

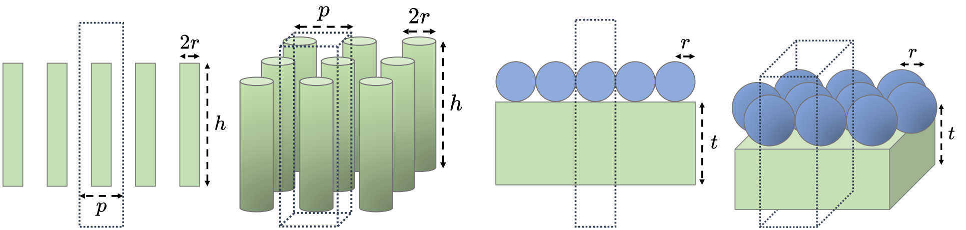


(a) Three-layer film

(b) Anti-reflective nanocones

Figure 2: Two- and three-dimensional nanophotonic structures. Different colors indicate different materials in each figure and a dotted region represents a simulation cell.

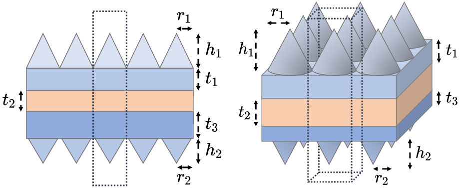
Nanophotonic Structures



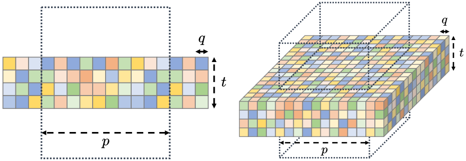
(a) Vertical nanowires (b) Close-packed nanospheres

Figure 3: Two- and three-dimensional nanophotonic structures. Different colors indicate different materials in each figure and a dotted region represents a simulation cell.

Nanophotonic Structures



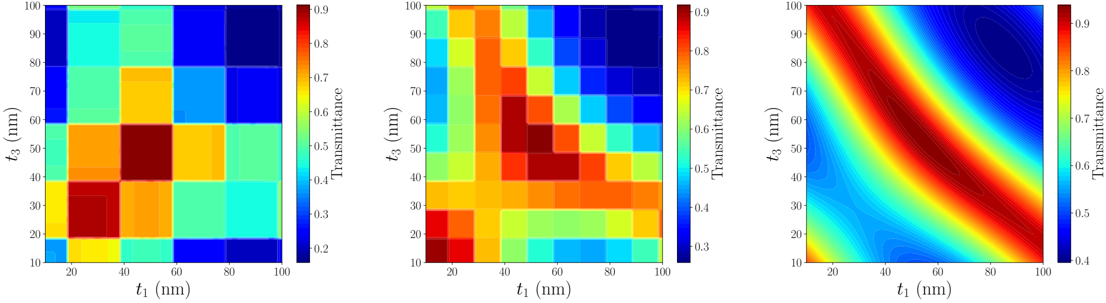
(a) Film with double-sided nanocones



(b) Combinatorial system with material blocks

Figure 4: Two- and three-dimensional nanophotonic structures. Different colors indicate different materials in each figure and a dotted region represents a simulation cell.

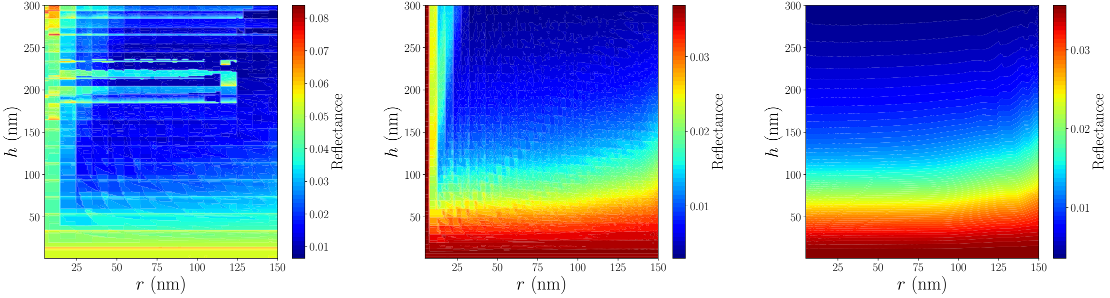
Visualization



(a) Low fidelity (b) Medium fidelity (c) High fidelity

Figure 5: Transmittance over parameters for the three-layer film made of $TiO_2/Ag/TiO_2$. Note that $t_2 = 3$ nm.

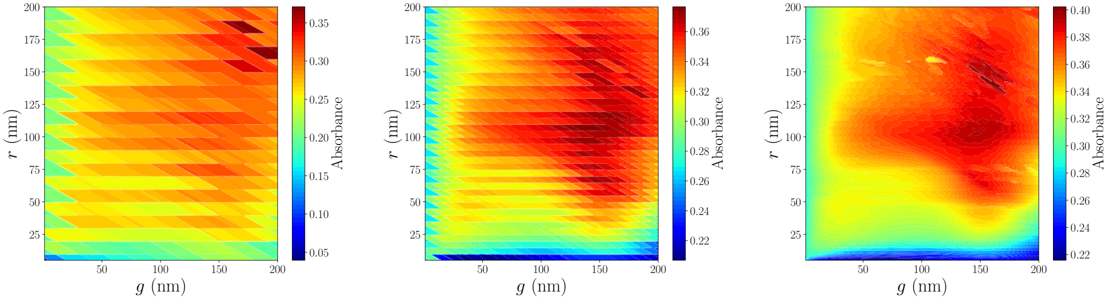
Visualization



(a) Low fidelity (b) Medium fidelity (c) High fidelity

Figure 6: Reflectance over parameters for the anti-reflective nanocones made of fused silica.

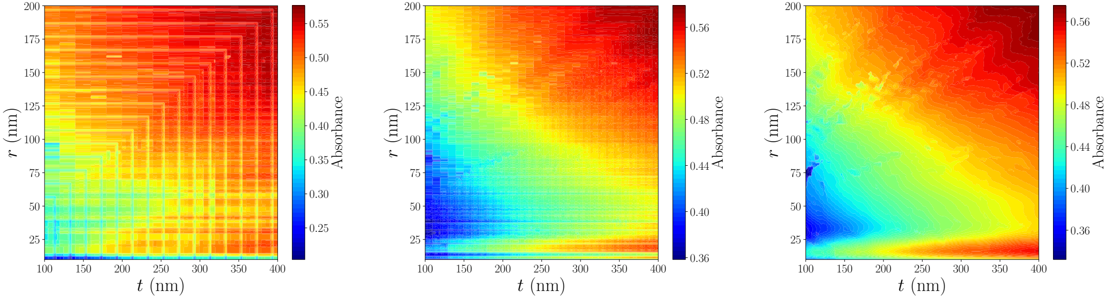
Visualization



(a) Low fidelity (b) Medium fidelity (c) High fidelity

Figure 7: Absorbance over parameters for the vertical nanowires made of cSi.

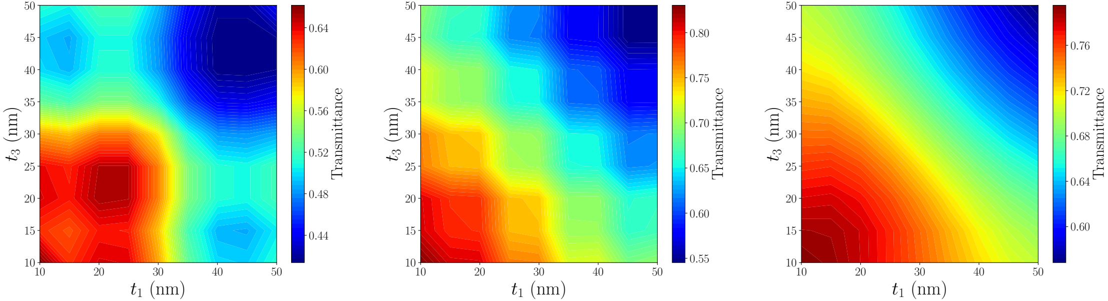
Visualization



(a) Low fidelity (b) Medium fidelity (c) High fidelity

Figure 8: Absorbance over parameters for the close-packed nanospheres made of cSi/TiO_2.

Visualization



(a) Low fidelity (b) Medium fidelity (c) High fidelity

Figure 9: Transmittance over parameters for the three-layer film with double-sided nanocones made of $TiO_2/Ag/TiO_2/TiO_2/TiO_2$. Note that $t_2 = 8$ nm, $r_1 = r_2 = 20$ nm, and $h_1 = h_2 = 50$ nm.

Visualization

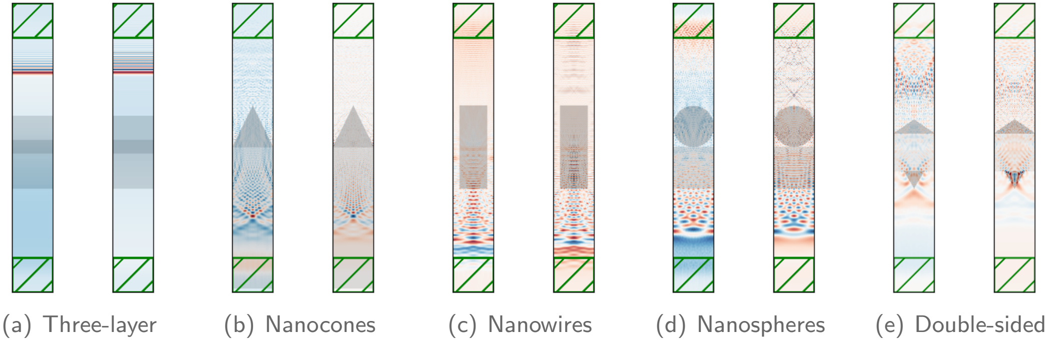
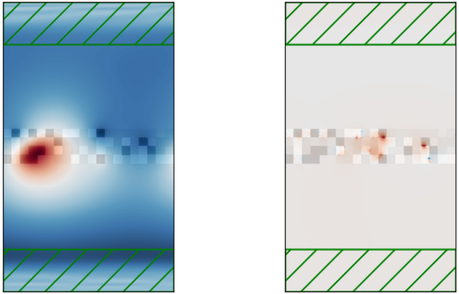


Figure 10: Examples of E-fields (left of each panel) and H-fields (right of each panel) out of plane for the structures studied in this work.

Visualization



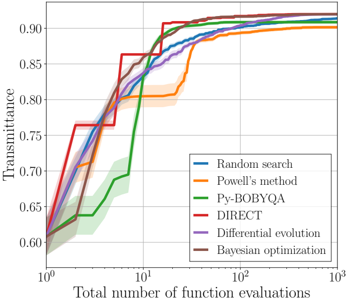
(a) Combinatorial system with material blocks

Figure 11: Examples of E-fields (left of each panel) and H-fields (right of each panel) out of plane for the structures studied in this work.

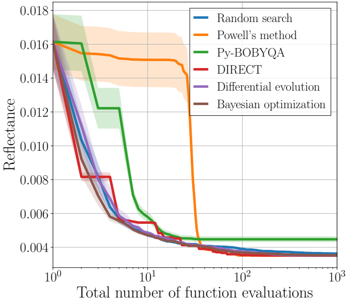
Optimization Modes

- Discretized Search Space Mode: In this mode, a search space is discretized with the increment specified in the paper. At each configuration a simulation is run and the outcome of the simulation is recorded.
- Surrogate Model Mode: Based on the dataset collected from the discretized search space, we fit a surrogate model. This allows us to evaluate any structural configuration in the search space using the trained surrogate model.
- Simulation Mode: Users can also directly run these simulations using our frameworks based on Meep and perform an optimization algorithm by conducting a simulation at every iteration.

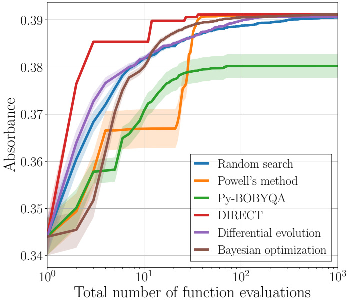
Experiments with the Surrogate Model Mode



(a) Three-layer film, $TiO_2/Ag/TiO_2$



(b) Nanocones, fused silica



(c) Nanowires, cSi

Figure 12: Results of experiments on nanophotonic structure optimization. Each experiment is conducted 50 times and the mean and standard error are depicted.

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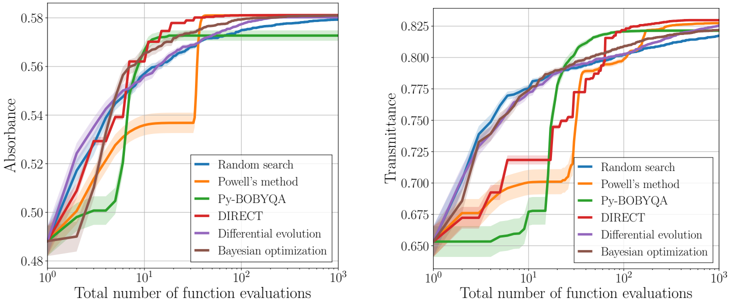
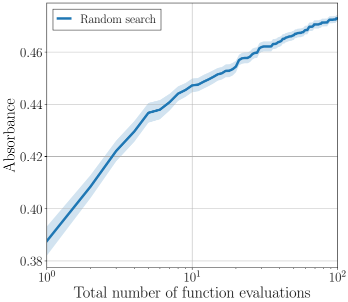
Experiments with the Surrogate Model Mode



(a) Nanospheres, cSi/TiO_2 (b) DS cones, $TiO_2/Ag/TiO_2$/–/–

Figure 13: Results of experiments on nanophotonic structure optimization. Each experiment is conducted 50 times and the mean and standard error are depicted.

Experiments with the Simulation Mode



(a) Combinatorial system

Figure 14: Results of experiments on nanophotonic structure optimization. Each experiment is conducted 50 times and the mean and standard error are depicted.

Conclusion

- We introduced several nanophotonic structures such as the three-layer film, anti-reflective nanocones, vertical nanowires, close-packed nanospheres, three-layer film with double-sided nanocones, and combinatorial system with material blocks.
- We devised a generic simulation scheme and pipeline for nanophotonic structure and parametric design simulations.
- We proposed datasets and benchmarks for modeling, simulating, and optimizing nanophotonic structures.
- We discussed the future directions, limitations, and societal impacts of our work in the paper.

Thank you!