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Global Phase Correction Improves Metalens Efficiency

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Abstract: We introduce a fast joint optimization of unit cells across the whole metasurface, exploiting interactions between nearby cells to produce a desired near-field profile and improving whole-lens focusing efficiency. © 2022 The Author(s)

In recent years, unit cell decomposition (UCD) has become the dominant design strategy for optical metalenses. UCD views a metalens as a grid of nano-structures that can be chosen independently to control the near field. UCD-designed lenses have demonstrated steadily improving focusing efficiencies, but fall short of theoretical predictions (and may be supplanted by freeform designs once simulation and fabrication challenges are resolved) [4]. One reason for the efficiency gap is that the electric field effect associated with an individual nano-structure is often based on periodic assumptions (the nano-structure identically tiles the plane), but when it is placed in a heterogeneous neighborhood of varied nano-structures, unmodeled coupling effects can substantially alter this response. Attempts to correct for this generally use extended supercell simulations in generate-and-test loops to find an alternate nano-structure that provides the desired near field in the context of its neighbors [2, 3]. These one-at-a-time search procedures are of limited effectiveness and are very expensive computationally, even when a pre-trained neural network is used as a proxy for the simulator.

We note that most simulator proxies are differentiable with regard to their inputs — not just their parameters — and thus provide an unexploited derivative for direct tuning of unit cell parameters. More powerfully, this opens the door to jointly optimizing all cells in the metalens to produce a desired near field distribution by solving a short sequence of linear equations, each with special structure enabling linear time and space complexity. Thus a metalens of millions of cells can be quickly optimized with modest computing resources. We apply this to the design of focusing TiO₂ nano-fin metalenses, previously designed according to the Pancharatnam–Berry (PB) phase theory, and obtain significant improvements in focusing efficiency. Our method is summarized in Fig. 1.

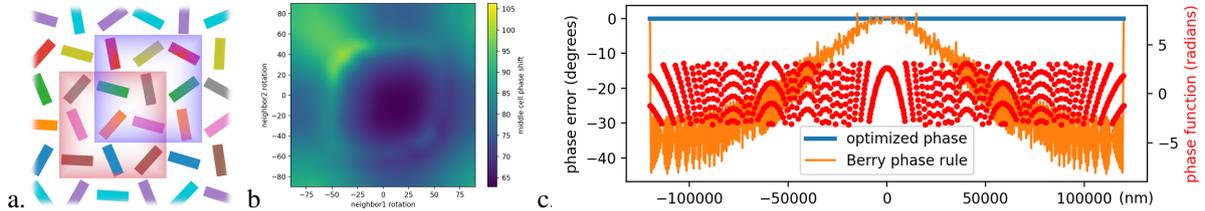


Fig. 1: Method overview: (a) A metalens is partitioned into densely overlapping neighborhoods, here 3×3 . (b) A differentiable function \hat{f} is fitted to supercell simulation data to predict the near field response of each neighborhood’s middle cell, here, a 2D slice through $\mathcal{L}\hat{f}$ as two neighbors are rotated, varying the phase of the average RCP electric field value over the middle cell by up $> 40^\circ$. (c) Design parameters for all cells are jointly optimized, here exactly matching the average phase shift of every cell to its target value for a focusing lens and increasing focal efficiency by $> 5\%$.

PB theory predicts that the phase shift offered by a suitably shaped waveguide is simply twice its planar orientation angle, i.e. $f(\theta) = 2\theta$. [1] did an extensive computational search in homogeneous LPA unit-cell simulations to find a nano-fin geometry that provides phase shifts as per PB and good transmission efficiency. In detailed FDTD simulations of heterogeneous supercells, we found that f has nonlinearities and dependencies on nearby nano-fins that can produce phase errors $> \pm 20^\circ$ (Fig. 1b). In addition, there are nano-fin geometries that provide superior transmission efficiency, but with larger deviations from ideal PB behavior. We use one such geometry here: $265 \times 95 \times 600\text{nm}$ TiO₂ nano-fins on SiO₂ substrate in a 325nm square grid. Generally, we observe deviations from PB phase when corners of adjacent nano-fins are close, indicating coupling effects, and when the phase shift varies substantially between adjacent fins, typically wherever a metalens provides nontrivial beam deflection. E.g., in Fig. 1c, the PB phase error grows to $> 40^\circ$ at the rim, though the *relative* phase error between adjacent cells is more modest, providing decent beam deflection. Nonetheless, this leaves room for optimization.

Optimization method: We approximate the unknown true phase function f^* with a differentiable interpolator $\hat{f}(\theta_1, \dots, \theta_d)$, fitted to simulation data of d -unit supercells. At design time, we then jointly optimize all design parameters $\Theta \doteq \{\theta_1, \dots, \theta_n\}$, $n \gg d$, to produce the desired near field via a Newton iteration applied to all overlapping d -unit neighborhoods on the metalens. Assuming that the near field at any point depends on a limited

neighborhood of the metalens, each iteration reduces to solving a banded linear system, which has $\mathcal{O}(n)$ time and space complexity. All examples in this paper, involving thousands of cells, completed in < 1 second.

We illustrate with 1D focusing lenses, then present the extension to the full planar case. For data, we simulated 3-cell supercells with different combinations of nano-fin orientations ranging from 0° to 180° in 10° increments. Each supercell was simulated via Maxwell equations on a 10nm grid, and the middle cell's near field measured at 33^2 XY points located 100nm beyond the fins. A simple barycentric interpolator \hat{f} was used to approximate the mapping (and its gradients) from local fin orientation angles θ_i to near field ϕ_i , e.g., $\phi_i \leftarrow \hat{f}(\theta_{i-1}, \theta_i, \theta_{i+1})$ in 1D. The interpolator essentially does piecewise linear interpolation between the 4 closest data points in angle space. For an n -cell metalens with cell parameters $\Theta \doteq \{\theta_j\}_{j=1..n}$ and target near field profile $\Phi^* \doteq \{\phi_i^*\}_{i=1..m}$, a correction $\Theta \leftarrow \Theta + \Omega$, $\Omega \doteq \{\omega_j\}_{j=1..n}$ is obtained by solving the linear system $\forall_i \sum_{j \in \mathcal{N}(i)} \partial_j \hat{f}_i(\{\theta_j\}) \omega_j = \hat{\phi}_i^* - \phi_i$, where $\mathcal{N}(i)$ is the set of cells that affect the electric field at the i th measurement point. We start with a baseline PB-phase-designed metalens and repeatedly correct, usually converging in 4–8 iterations.

Results: When target Φ^* is the phase of the *average* electric field value above a unit cell, the linear system is square and exactly solvable, such that the method yields a set of orientations that produces zero average phase error (Fig. 1c). Although based on a coarse sampling of the near field, this typically yields $> 8\%$ improvements in focusing efficiency of high-NA metalenses in both Rayleigh–Sommerfeld far-field calculation from \hat{f} and in detailed FDTD simulations (Fig. 2a).

. When target Φ^* is the desired phase distribution of electric field sampled every 10nm, the linear system is over-constrained and is solved in an minimum-squared-error sense, revealing residual phase errors at the edges of each cell that grow with distance from the lens center (Fig. 2b). This solution has more fidelity to the actual physics than the average phase solution, and therefore exhibits superior focusing efficiency when both are simulated at a 10nm level of detail. Finally, when target Φ^* is the full complex-valued electrical field, there is small further gains in focusing efficiency, typically $< 0.2\%$.

In general, rapid changes in the target phase function seem to be problematic for UCD. Good unit cell sizes necessarily undersample the rapidly changing high-NA focusing lens phase function, which can vary $> 150^\circ$ per cell near the rim; this may argue for designing the outer annulus of high-NA metalens via freeform methods.

Extension to 2D: The method extends directly to 2D arrays of unit cells, and fortunately does not require a much larger set of supercell simulations for interpolation data, which might be expected due to the combinatorics of possible neighbor choices. We found that for 3×3 supercells sampled randomly from focusing metalenses, the near field of the middle cell is well predicted by linear regression on the near fields of its central 3×1 and 1×3 subregions (for which we already have a validated \hat{f}_{1D}), scaled by the sines and cosines of the intended deflection direction. The resulting \hat{f}_{2D} has an average relative error of $\approx 10\%$, reducing the near field prediction residual by $> 85\%$ compared to the PB phase prediction, and whole-lens optimization preserves $> 79\%$ of this improvement. This accords with that the expectation that f_{2D} is a weighted superposition of many f_{1D} functions, in which the horizontal and vertical components dominate.

Summary: We introduced a fast optimizations that simultaneously tunes all unit cells to improve the near field distribution, mainly by correcting for interactions between nearby cells. This improves the focusing efficiency of high-NA metalenses by 5-9%, as validated in high-resolution FDTD simulations.

References

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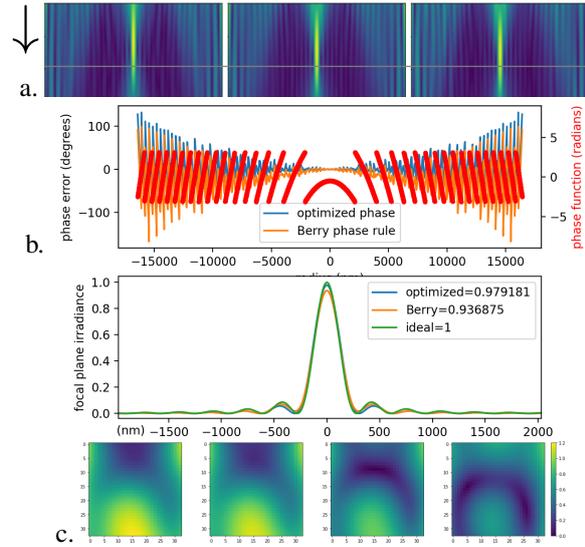


Fig. 2: (a) Propagation fields from full FDTD simulations of small NA=0.937 metalenses designed via (left to right): the PB rule; phase optimization (+7.8% focal efficiency); and combined phase and intensity optimization (+8.1%). Note the improved focal depth. (b) An NA=0.8 lens optimized at near field points every 10nm shows that error can be minimized but not zeroed, because the target phase changes too rapidly within distal cells. The zoomed far field intensity distribution shows improved focusing efficiency. (c) Error predicting a 3×3 supercell near field distribution from: PB phase; the closest 3-supercell; an average of 2 3-supercells; and regression. Darker is better.