

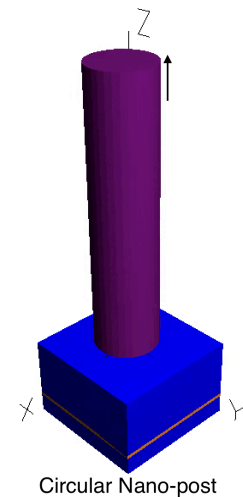
# Supplement:

## Contrary to widespread belief, the Fresnel zone plate outperforms the metalens at high NA.

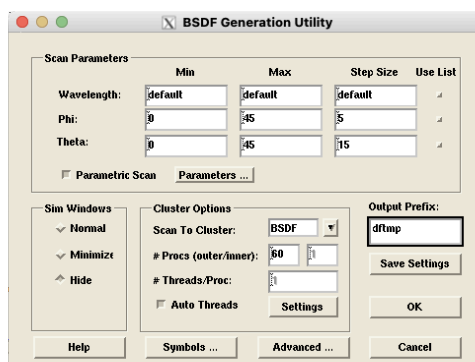
### 1. Metalens design:

The design and simulation of the metalens began with the development of a meta-atom, the fundamental building block of the metalens structure. Meta-atoms are nano-sized cells, each with specific dimensions and geometries, arranged in precise patterns to create the metalens. These meta-atoms exhibit unique optical properties determined by the Locally Periodic Approximation (LPA), where the pitch size is subwavelength ( $\Lambda < \lambda$ ). Each meta-atom on the metalens contributes to the desired phase shift necessary for focusing light.

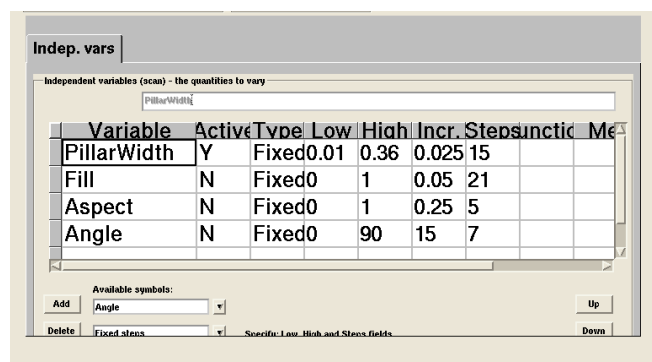
For this study, we implemented a circular nano-post pattern in which each meta-atom was designed as a cylindrical dielectric post mounted on a  $0.2\ \mu\text{m}$  glass substrate. Assessing the transmission and reflection characteristics of each meta-atom was crucial for optimal metalens performance. Under the LPA approach, the transmission and reflection coefficients of a single unit cell could be calculated using periodic boundary conditions in the transverse direction and open boundary conditions in the longitudinal direction.



A Bidirectional Scattering Distribution Function (BSDF) Generation Utility was employed using RSoft FullWAVE FDTD to model light interaction with the meta-atom. The BSDF characterized scattering behavior by defining reflection and transmission across multiple directions, taking into account variables such as incident angle, wavelength, and polarization. During the BSDF generation, a parametric scan was performed across meta-atom cylinder lengths ( $0.01\ \mu\text{m}$  to  $0.50\ \mu\text{m}$ ) and widths ( $0.0102\ \mu\text{m}$  to  $0.36\ \mu\text{m}$ ) to build a comprehensive scattering profile.



BSDF generation utility settings (RSoft)



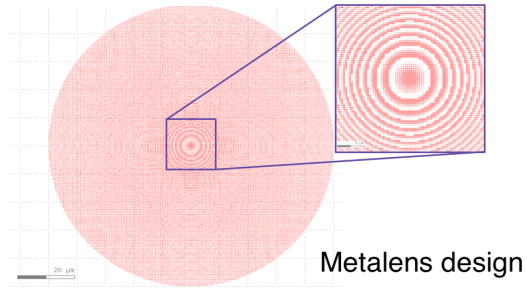
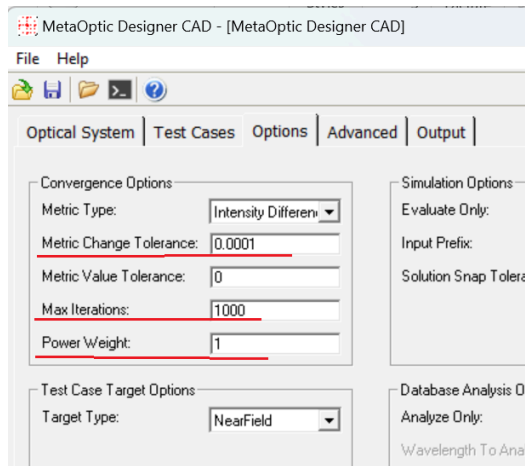
BSDF Parametric scan

The compiled BSDF library was used to determine the optimal lens design with desired target in MetaOptic Designer (MOD), an inverse-design tool from Synopsys. Using this BSDF data, MOD automated the metalens design, optimizing the configuration to achieve the target optical performance. This iterative design approach ensured the most effective arrangement of meta-atoms, tailored to desired specifications through an inverse-design process. There is a parameter of period, which is the array of atoms. MOD uses the meta-atom period as a computation grid, so that the XY resolution is fixed by the lattice period. The period, or spacing of the meta-atoms, of the lens was set to  $0.3\ \mu\text{m}$  as this was found to be optimal. The phase profile of the meta-atoms for a metalens is typically defined as:

$$\Psi(x, y, \lambda) = -\frac{2\pi}{\lambda} (\sqrt{x^2 + y^2 + F^2} - F)$$

The maximum meta-atom width ( $0.36\ \mu\text{m}$ ) exceeded the period ( $0.3\ \mu\text{m}$ ), leading to overlapping meta-atoms in the metalens structure. The metalens was designed with a diameter of  $100\ \mu\text{m}$  and a focal length of  $9.89\ \mu\text{m}$ , resulting in a numerical aperture (NA) of 0.98, optimized to focus 647 nm wavelength light. The dielectric material used has a refractive index of 1.5039, while the glass substrate has a refractive index of 1.4566.

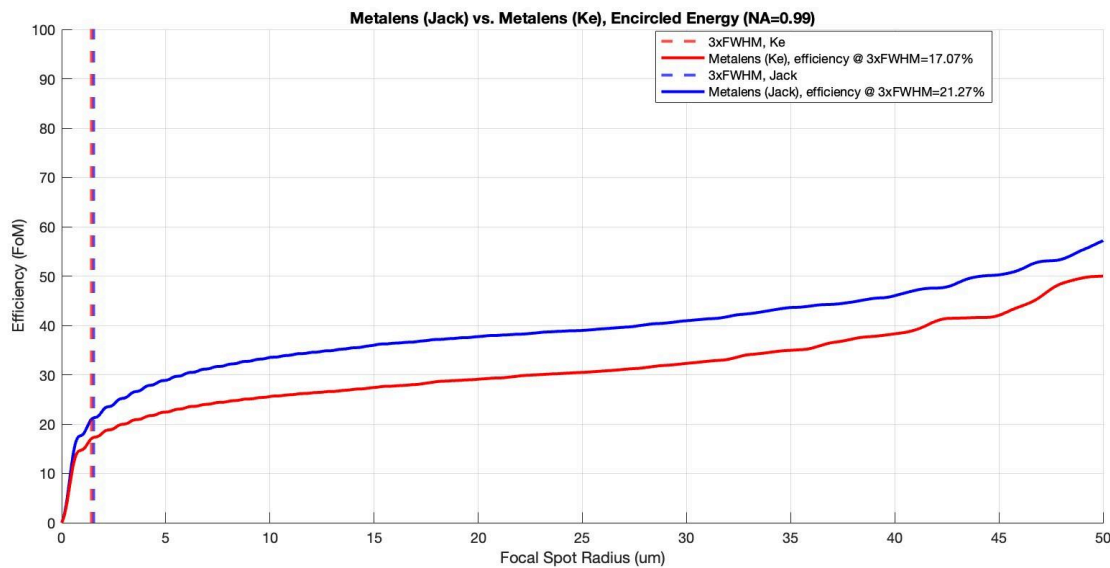
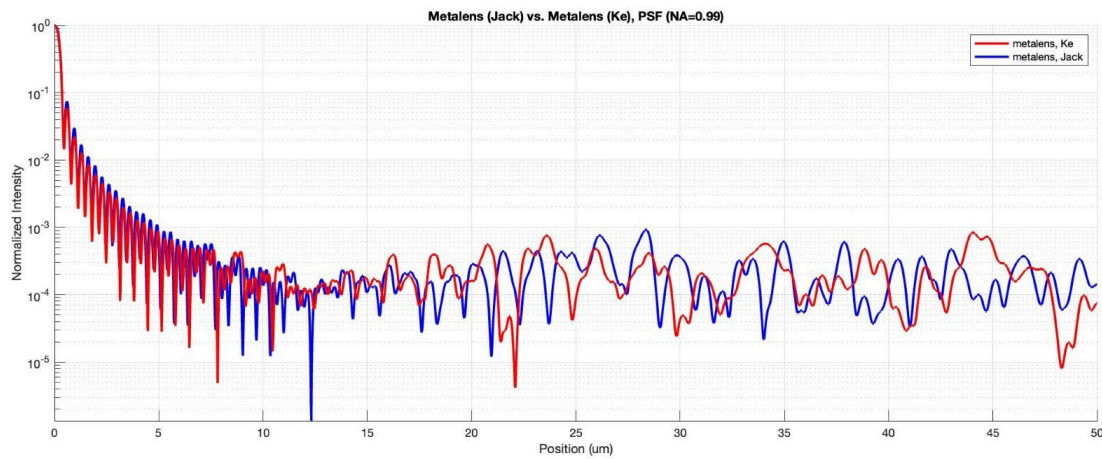
The generated metalens .ind file from MetaOptic Designer (MOD) was subsequently exported to RSoft FullWAVE FDTD for comprehensive validation through a full 3D simulation. Additional details are provided below.



## 2. Additional Metalens Design:

To evaluate the effectiveness of our metalens design relative to other configurations, we collaborated with Ke Liu (ke.liu2@synopsys.com), an Applications Engineer at Synopsys, to

create an additional design based on our parameters (Diameter = 100  $\mu\text{m}$ , Focal Distance = 9.89  $\mu\text{m}$ , NA = 0.98, Wavelength = 0.647  $\mu\text{m}$ , Refractive Index = 1.5039). Ke developed a metalens with a period of 0.325  $\mu\text{m}$  and meta-atom pillar widths ranging from 0.0102  $\mu\text{m}$  to 0.3  $\mu\text{m}$ . As his period was larger than the widest pillar, this alternative design avoided overlapping pillars, unlike our original configuration. Both metalens designs were then simulated under identical conditions (details provided below), followed by an in-depth analysis comparing their performance. The primary metrics assessed were the point spread function (PSF) and encircled energy in the XZ plane. The analysis concluded that our original design, with a period of 0.3  $\mu\text{m}$  and maximum pillar width of 0.36  $\mu\text{m}$ , outperformed the alternative by exhibiting superior focusing efficiency.



### 3. Design and simulation of the Fresnel zone plate (FZP):

The parabolic phase shift was calculated for the FZP design. The parabolic phase shift represents the difference in the optical path length between a point at radial distance  $r$  from the optical axis and the central point at the optical axis (where  $r = 0$ ). This phase shift is critical for accurately modeling the behavior of light in the FZP. The parabolic phase shift, denoted as parabolic shift1, is given by

$$\text{parabolic shift} = \sqrt{r^2 + f_0^2} - f_0$$

where  $f$  is the focal length, and  $r$  is the radial distance from the optical axis. This equation represents the difference between the actual path length of light traveling along a parabolic surface and the straight-line path along the axis. To determine the maximum phase shift across the entire lens or aperture, we calculate the shift at the edge, where the radial distance is  $D/2$  (half of the lens diameter). The maximum parabolic shift, max parabolic shift1, is given by

$$\text{max parabolic shift} = \sqrt{\left(\frac{D}{2}\right)^2 + f_0^2} - f_0$$

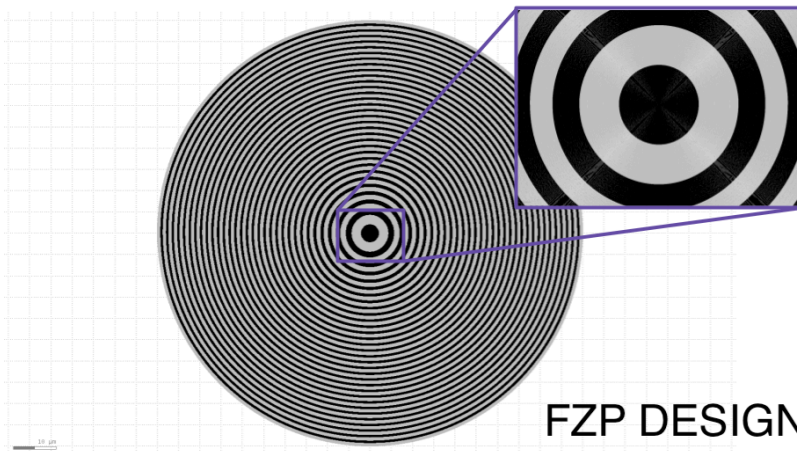
where  $D$  is the total diameter of the lens. Next, we normalize the difference between the maximum parabolic shift and the current parabolic shift to account for the refractive index of the material. This normalization is essential for describing the propagation of light within a medium with refractive index  $n_{\text{refr}}$ , and is expressed as:

$$x_0 = \frac{\text{max parabolic shift} - \text{parabolic shift}}{n_{\text{refr}}}$$

Finally, to ensure that the phase shift remains within a physically meaningful range, typically within one wavelength, we apply a modular operation. This operation constrains the shift to within the wavelength  $\lambda$ , which is critical for optical interference effects. The adjusted phase shift is given by

$$x_0 = \frac{(x_0 \cdot (n_{\text{refr}} - 1)) \bmod \lambda_0}{n_{\text{refr}} - 1}$$

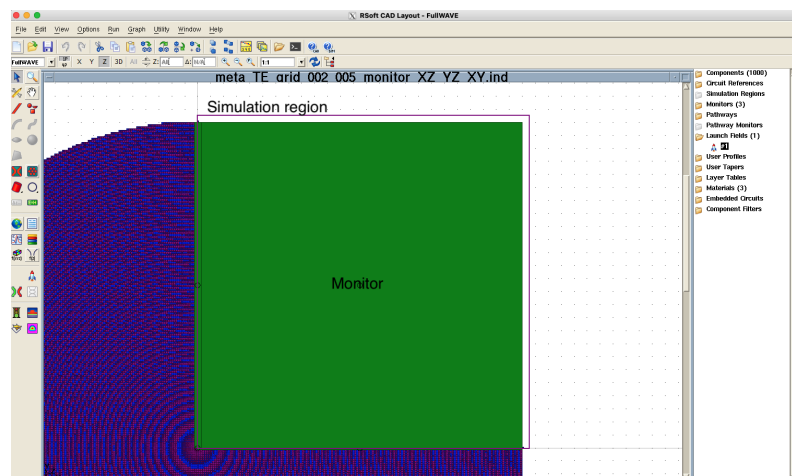
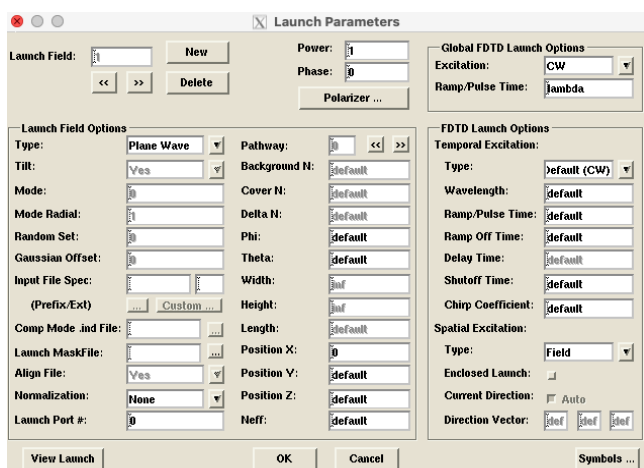
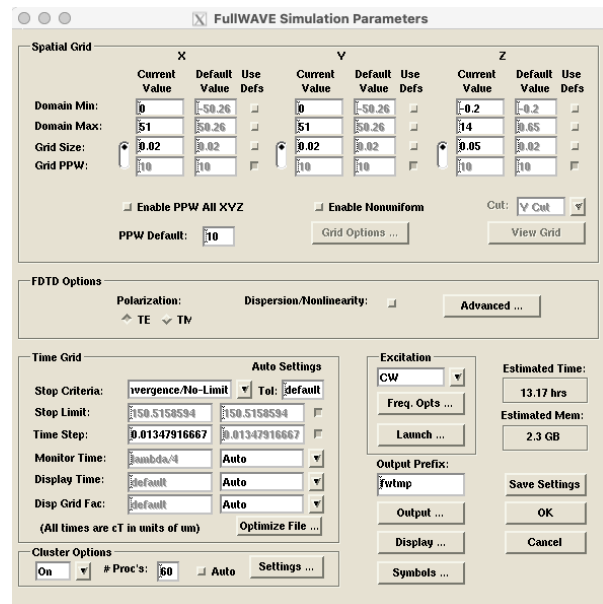
This sequence of equations describes how the parabolic phase shift is calculated for our FZP. The FZP structure resulted in 4892 total rings, minimum Ring Width = 0.0102  $\mu\text{m}$  and max Ring Height = 1.28  $\mu\text{m}$ .



## Simulation:

RSoft FullWAVE is a commercial software tool designed for comprehensive optical simulations based on the finite-difference time-domain (FDTD) method, ideal for analyzing light behavior in complex photonic structures. All simulations were conducted in 3D; however, only the first quadrant of each lens was modeled using radial calculation with assumed symmetry to reduce time and computational resources.

The FDTD technique in RSoft was applied with a grid resolution of  $0.02\text{ }\mu\text{m}$  in the  $x$  and  $y$  directions and  $0.05\text{ }\mu\text{m}$  in the  $z$  direction (approximately 32 points per wavelength). The FDTD algorithm can detect metalens features with a minimum of five grid points per feature (with 10 being an empirical ideal). At the current grid size, features as small as  $0.02\text{ }\mu\text{m}$  would only register one grid point, which is insufficient. Therefore, this setup effectively detects features down to a size of  $0.1\text{ }\mu\text{m}$  (i.e.,  $0.02 \times 5 = 0.1\text{ }\mu\text{m}$ ). To accurately simulate features as small as  $0.01\text{ }\mu\text{m}$ , the grid would need to be reduced to  $0.002\text{ }\mu\text{m}$  in the  $x$  and  $y$  directions. However, such a setup would demand extensive computational resources, estimated at 30 days and 188 GB of RAM. The FDTD computation time scales with  $N^4$ , where  $N$  is the total number of grid points, reflecting an additional time-dimension complexity in 3D FDTD simulations. The simulation region was confined within boundaries of  $51 \times 51 \times 14\text{ }\mu\text{m}^3$ , surrounded by a Perfectly Matched Layer (PML) with a thickness of  $1\text{ }\mu\text{m}$  to minimize boundary reflections. Three monitors were positioned on the XZ, YZ, and XY planes to measure energy density and electric field components ( $E_x$ ,  $E_y$ , and  $E_z$ ). A plane wave with a wavelength of  $647\text{ nm}$  and transverse electric (TE) polarization was introduced at normal incidence. Each metalens simulation was run on 60 processors with 2 TB of RAM and completed in approximately 8 hours, whereas the Fresnel Zone Plate (FZP) simulations took around 72 hours to conclude.



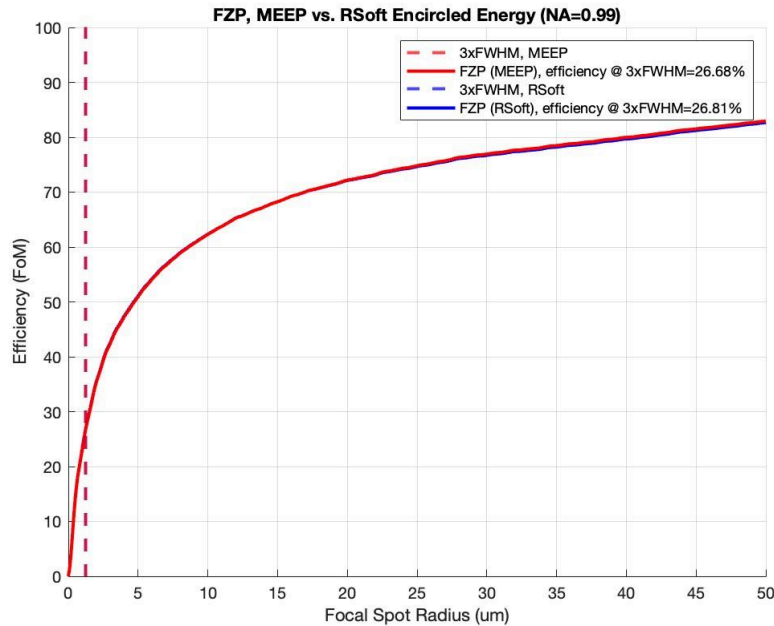


### Validation:

To validate our results, we conducted simulations using an additional FDTD software, MEEP (MIT Electromagnetic Equation Propagation). MEEP is an open-source FDTD tool designed for simulating light behavior in complex photonic structures, similar to RSoft FullWAVE. Both RSoft FullWAVE and MEEP are widely used in photonics research, and theoretically, they should produce equivalent results under identical simulation structures, parameters, and boundary conditions. We verified this equivalency by simulating an XZ slice of the Fresnel Zone Plate (FZP) in both softwares. In each simulation, a monitor was positioned in the XZ plane to measure energy density within the region. Following the simulations, we conducted a detailed metric analysis of the results using MATLAB. Both MEEP and RSoft produced nearly identical focal point shapes and focal shifts: MEEP recorded a focal shift to  $9.5470\text{ }\mu\text{m}$ , while RSoft measured  $9.5484\text{ }\mu\text{m}$ . Additionally, both simulations showed comparable depth of focus (DOF) values, with RSoft returning  $0.74053\text{ }\mu\text{m}$  and MEEP showing  $0.74058\text{ }\mu\text{m}$ . Radial intensity results also aligned closely, each displaying a full-width at half-maximum (FWHM) of  $0.41294\text{ }\mu\text{m}$ . The encircled energy and figure of merit (FoM) metrics were similarly consistent between the two tools, with RSoft yielding an FoM of 26.68 and MEEP reporting 26.81. The encircled energy plots from both simulations overlapped almost perfectly, indicating highly reliable results across both software platforms.

Metric	RSoft	MEEP
Efficiency (FoM)	26.68	26.81
FWHM ( $\mu\text{m}$ )	0.41294	0.41294
DOF ( $\mu\text{m}$ )	0.74053	0.74058
Focal Distance ( $\mu\text{m}$ )	9.5470	9.5484

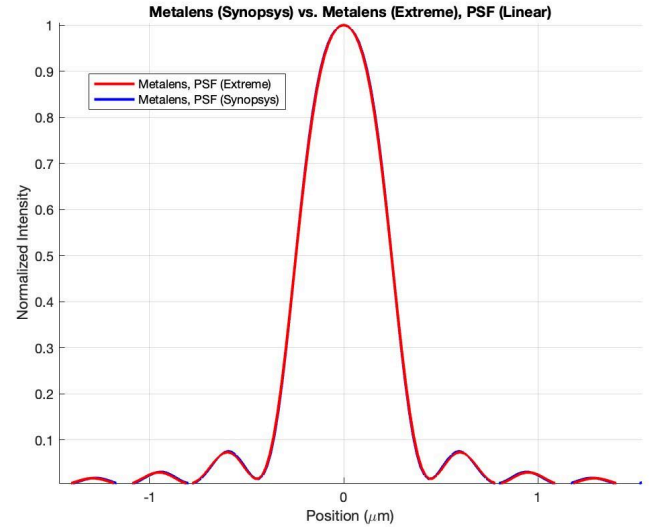
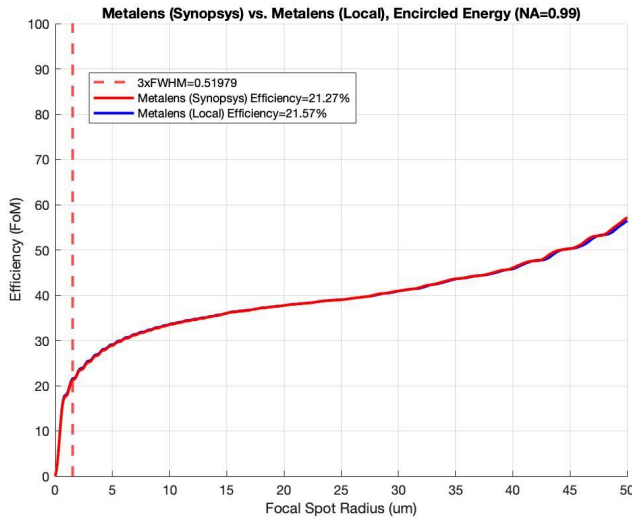
MEEP vs. RSoft Results (Table 1)



As shown in all figures and tables, the results from RSoft and MEEP simulations are nearly identical when simulating the same lens under equivalent FDTD conditions. Metric variations between the two software platforms were minimal, with differences of less than  $0.002\ \mu\text{m}$  in focal distance, depth of focus (DOF), focal shift, and FWHM. Efficiency varied by only 0.17%, and intensity profiles and focal shapes were virtually indistinguishable. Thus, we conclude that MEEP and RSoft produce sufficiently consistent results, confirming the accuracy of the FZP simulation results, as they have been successfully reproduced in two different FDTD software platforms.

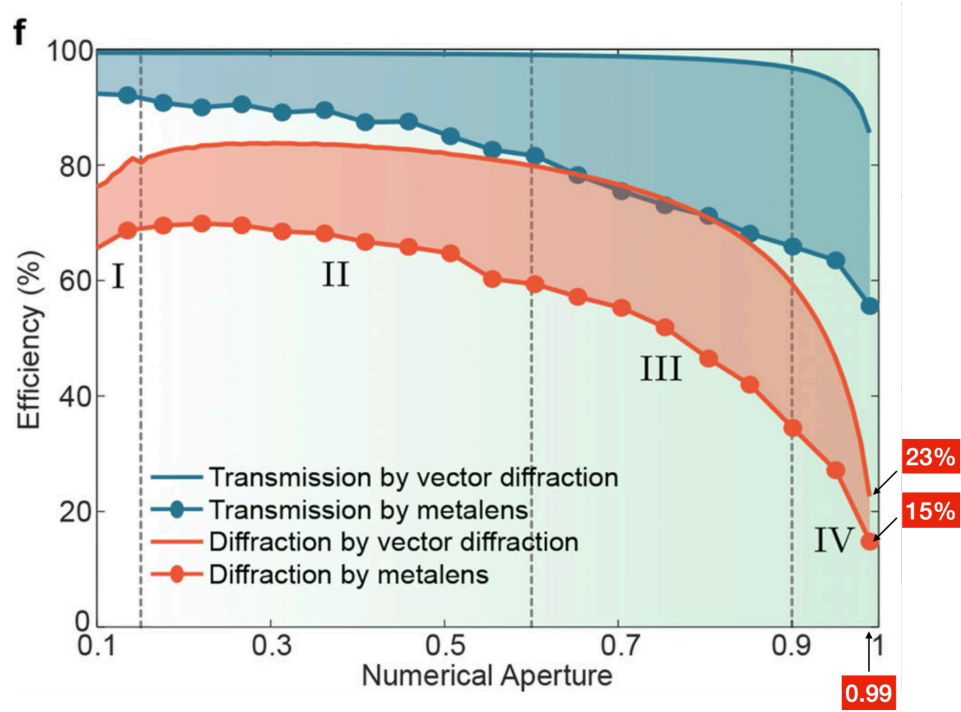
Beyond validating the FZP, the metalens simulation results were independently verified using a different approach. The metalens design was simulated by two individuals on two separate systems, and the outcomes were compared. Our simulation was conducted on a server with 60 cores and 2 TB of RAM, while the second simulation was performed by Ke Liu (ke.liu2@synopsys.com), an Applications Engineer at Synopsys (developer of RSoft), on a system with 16 cores and 120 GB of RAM. Both simulations adhered to the same protocols and parameters, as detailed above. The results were consistent across both setups, thereby validating the metalens simulation outcomes.

Metric	Metalens (Local)	Metalens (Synopsys)
Efficiency (FoM)	21.57	21.27
FWHM ( $\mu\text{m}$ )	0.51465	0.51465
DOF ( $\mu\text{m}$ )	0.70110	0.70090
Focal Distance ( $\mu\text{m}$ )	9.89	9.89



#### 4. Numerical simulations from Ref. 11 in main text:

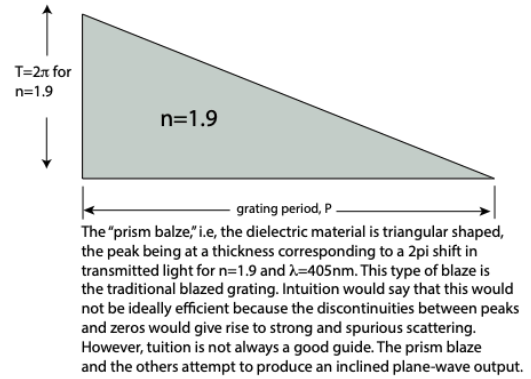
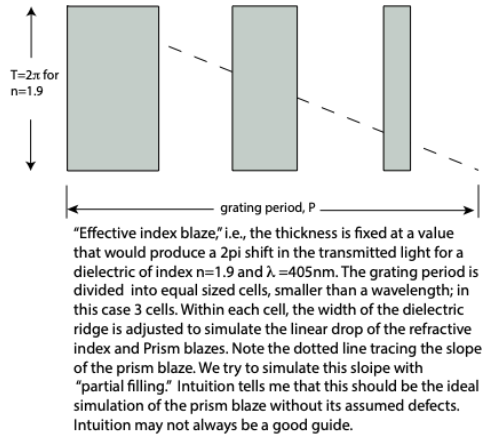
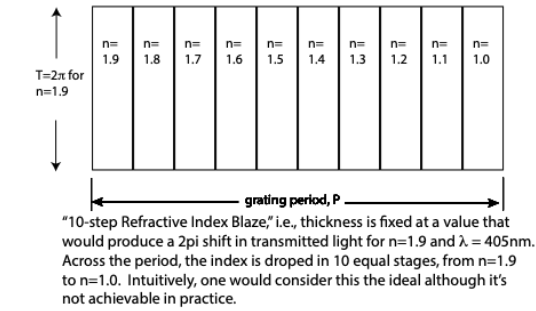
We reproduce Fig. 2f from Ref. 11 below to indicate the calculated diffraction efficiencies therein. We further confirmed with the authors of the paper that these plots are created assuming a focal-spot radius of 3 x FWHM.



## 5. Simulation of gratings using Gsolver.

The details of the grating geometries are summarized below.





Note: The widths of the ridges in the effective-index blaze, i.e., the filling factor, can be chosen based on the slope of the dotted line, let's call this the intuitive method; or one can use a genetic algorithm (GA) to choose the widths and positioning of the ridges. The latter GA approach invariably produces a higher diffraction efficiency than the intuitive method.

We thus identify 2 modes of the Effective-Index Blaze: The intuitive effective-index mode (IEIM) and the Genetic Algorithm effective-index mode (GAEIM). Note that one can claim that GAEIM is a close cousin to, and may be more effective than, the widely used and touted inverse design approach.

Table below summarizes the simulated efficiencies.

NA	blazed / TE	meta / TE	blazed / TM	meta / TM
0.998996	11%	2%	13%	0%
0.969071	44%	9%	44%	1%
0.940886	56%	13%	53%	3%
0.914294	64%	17%	59%	5%
0.889164	71%	21%	64%	7%
0.865378	75%	25%	68%	9%
0.842832	79%	29%	70%	11%
0.821431	81%	32%	73%	14%
0.80109	83%	35%	74%	16%
0.781731	84%	38%	75%	19%
0.763287	84%	40%	76%	21%
0.745692	84%	43%	76%	23%
0.728891	81%	45%	74%	25%
0.71283	78%	47%	73%	27%

0.697461	75%	48%	72%	29%
0.682742	72%	50%	71%	31%
0.66863	68%	51%	68%	33%
0.65509	62%	52%	65%	35%
0.642088	56%	53%	62%	36%
0.629592	49%	53%	57%	38%
0.617573	42%	55%	53%	38%

## 6. Validation of grating simulations using MEEP.