Optimization under uncertainty for the Helmholtz equation with application to PNJ configuration

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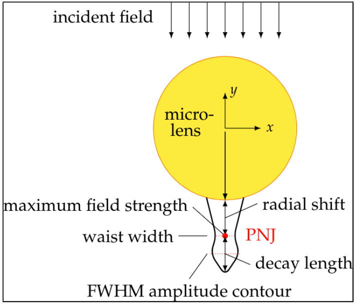
AIP23: MS51-2 7th of September 2023

Outline

- What is a PNJ, background, and motivation
- The deterministic PNJ design
- PNJ design under manufacturing uncertainty
- Towards topology optimization of PNJ lens design

What is a photonic nanojet (PNJ)

- A PNJ is a highly focused light beam formed in the near field of a micrometer-sized dielectric lens illuminated by a light wave



Schematic illustration of Photonic Nanojet (PNJ) [Karamehmedović et al., 2022]

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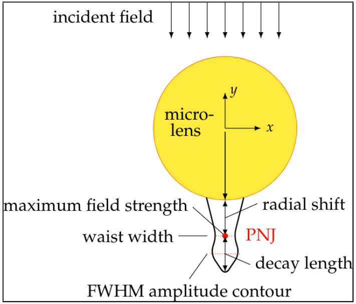
- PNJ enables imaging of particles beyond the diffraction limit $d_{\text{limit}} = \lambda/(2NA)$, Numerical Aperture (NA) ≤ 1.6



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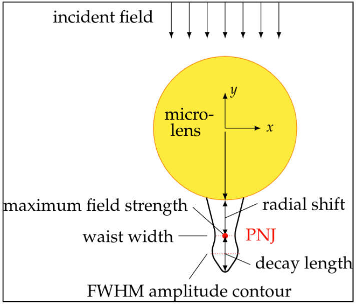
- PNJ enables imaging of particles beyond the diffraction limit $d_{\text{limit}} = \lambda/(2NA)$, Numerical Aperture (NA) ≤ 1.6
- Numerous applications [Karamehmedović and Glückstad, 2023, Darafsheh, 2021]:
  - super-resolution optical microscopy
  - nanoparticle detection, counting, and manipulation (optical tweezers) [Hansen et al., 2023]



Schematic illustration of Photonic Nanojet (PNJ) [Karamehmedović et al., 2022]

PNJ design in the literature

Design of PNJ with desired properties (e.g. position, size and shape) has been investigated in numerous studies

- Most studies consider homogeneous lenses and achieve control via changing the lens shape [Chen et al., 2021b, Hengyu et al., 2015]

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- PNJ steering and nano-particle detection in the literature [Karamehmedović et al., 2022, Karamehmedović and Glückstad, 2023, Karamehmedovic and Hansen, 2023]

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- PNJ steering and nano-particle detection in the literature [Karamehmedović et al., 2022, Karamehmedović and Glückstad, 2023, Karamehmedovic and Hansen, 2023]
- Limited (possibly non-existent) studies that account for the lens manufacturing/illumination imprecision

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- Systematic approach to design/control PNJ properties (location & intensity)

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- Achieved via finding optimal heterogeneous lens profile
  - This provides flexibility in design
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- Applied to PNJ design and steering (many lenses)

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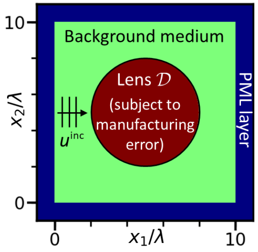
Helmholtz (Forward)

Helmholtz equation

$$\Delta u^{\text{sca}} + k^2(x) u^{\text{sca}} = (k_0^2 - k(x)^2) u^{\text{inc}} \quad \text{in } \mathbb{R}^d \tag{1}$$

+ Sommerfeld radiation condition (approximately modeled by PML)

- $d = 2, 3$
- Incident wave $u^{\text{inc}} = e^{ik_0 x.b}$, b is the wave direction.
- u^{sca} is the scattered wave
- $k_0 = \omega / c_0$ is the background medium wave number
- $k(x) = \omega / c(x) = k_0 n(x)$ is the spatially varying wave number ($= k_0$ outside the lens)
- $n(x)$ is the refractive index ($= 1$ outside the lens)



Design Problem Formulation

Design objective $\mathcal{Q}$

$$\mathcal{Q}(u^{\text{tot}}(\tau)) = \frac{1}{2}\int_{\mathbb{R}^d} \delta_{x_{\text{PNJ}}}(x)\left(|u^{\text{tot}}(\tau)|^2 - A_{\text{PNJ}}^2\right)^2 \tag{2}$$

- $u^{\text{tot}} = u^{\text{sca}} + u^{\text{inc}}$
- u^{tot} is the total wave field
- $\delta_{x_{\text{PNJ}}}(x)$ is the Dirac delta at $x_{\text{PNJ}} \in \mathbb{R}^d$
- A_{PNJ} is the desired PNJ amplitude
- $\tau(x)$ is the design variable ($k(x) = k_0 + e^{\tau(x)}\chi_{\mathcal{D}}(x)$)
- $\chi_{\mathcal{D}}$ is the characteristic function with support on the lens $\mathcal{D}$

Optimization

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- The gradient is computed using the adjoint based method
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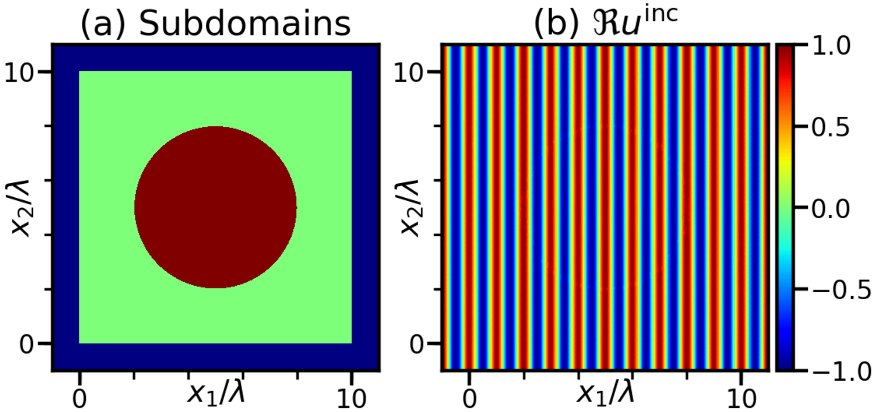
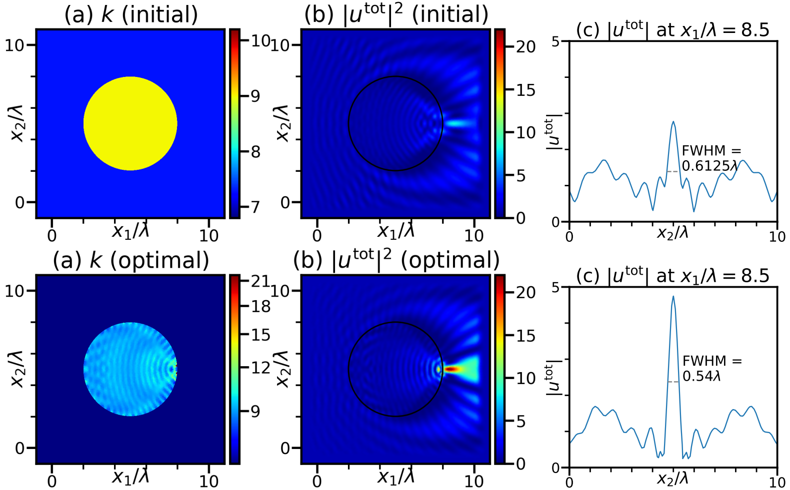
- We use the software tool: Stochastic Optimization under high-dimensional Uncertainty in Python (SOUPy)

Results: Setup and Incident Wave



- $u^{\text{inc}} = e^{ik_0 x.b}$

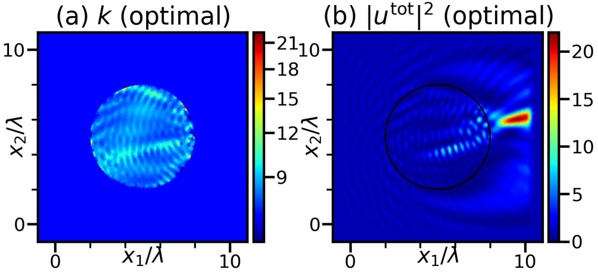
Results: Deterministic Optimization



- $x_{\mathrm{PNJ}} = (8.5, 5)$, $A_{\mathrm{PNJ}} = 20$
- $|u^{\mathrm{tot}}|$ is measured in V/m and k is measured in m^{-1}

Results: Deterministic Optimization (Angular Shift)

$A_{\text{PNJ}} = 20$, $x_{\text{PNJ}} = (9.5, 6)$



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Design Problem Formulation (Uncertainty)

Design objective $\mathcal{Q}$

$$\mathcal{Q}(u^{\text{tot}}(\tau,\zeta)) = \frac{1}{2}\int_{\mathbb{R}^d} \delta_{x_{\text{PNJ}}}(x)\left(|u^{\text{tot}}(\tau,\zeta)|^2 - A_{\text{PNJ}}^2\right)^2 \tag{3}$$

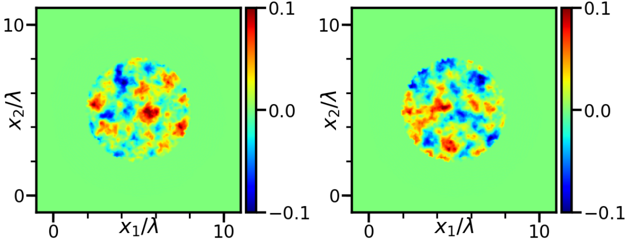
- ζ is the manufacturing noise (random field)
- $k = k_0 + e^{\tau+\zeta}\chi_{\mathcal{D}}$

Manufacturing Error

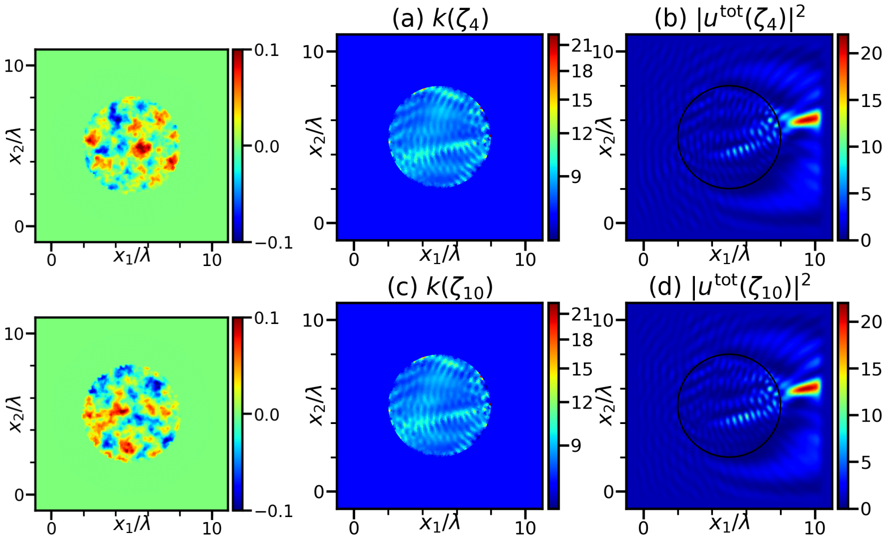
Matérn class Gaussian random field ζ

- $\zeta \sim \mathcal{N}(0, \mathcal{C})$
- $(\delta I - \gamma \Delta)^{\alpha/2} \zeta(x) = w(x)$ in $\mathcal{D}$
- $\nabla \zeta \cdot n = 0$ on $\delta \mathcal{D}$

- $w(x)$ is white noise
- The choice of δ and γ dictates the variance and the correlation length
- $\mathcal{C}$ is the covariance operator
- $\alpha > d/2$
- Here, $\alpha = 2$, $\gamma = 2.5$, and $\delta = 25$



Results: Deterministic Optimization (Effect of Noise)



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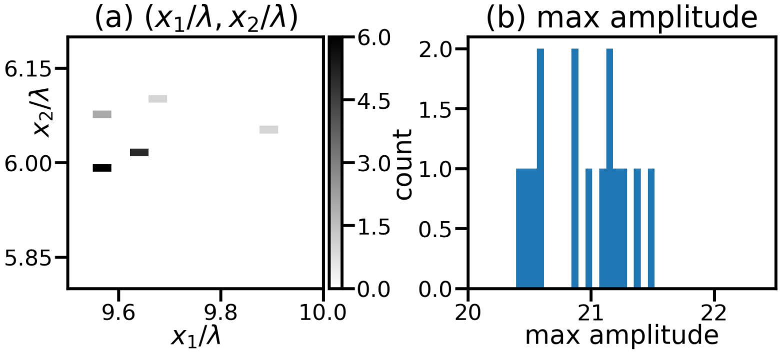


Optimization under Manufacturing Uncertainty

design objective revisited, risk-averse mean-variance formulation

$$\mathcal{J}(\tau) = \mathbb{E}_\zeta[\mathcal{Q}(\tau,\zeta)] + \beta_V \mathrm{Var}_\zeta[\mathcal{Q}(\tau,\zeta)] + \beta_P P(\tau) \tag{4}$$

- $\mathbb{E}_\zeta$ and Var_ζ denotes expected value and variance, respectively.
- $P(\tau) = \int_\mathcal{D} |\tau(x)| dx \approx \int_\mathcal{D} (\tau^2(x) + \epsilon)^{\frac{1}{2}} dx$, L1 penalty term
- β_V and β_P are weights for the variance and the regularization terms.

Approximation of the Optimization Problem (SAA)

- **Sample average approximation (SAA)**
- Taylor approximation

Mean and variance approximation

$$\mathbb{E}_\zeta[\mathcal{Q}(\tau, \zeta)] \approx \bar{\mathcal{Q}} := \frac{1}{M} \sum_{m=1}^{M} \mathcal{Q}(\tau, \zeta_m) \tag{5}$$

$$\mathrm{Var}_\zeta[\mathcal{Q}(\tau, \zeta)] = \mathbb{E}_\zeta[\mathcal{Q}^2(\tau, \zeta)] - \mathbb{E}_\zeta[\mathcal{Q}(\tau, \zeta)]^2 \approx \frac{1}{M} \sum_{m=1}^{M} \mathcal{Q}^2(\tau, \zeta_m) - \bar{\mathcal{Q}}^2 \tag{6}$$

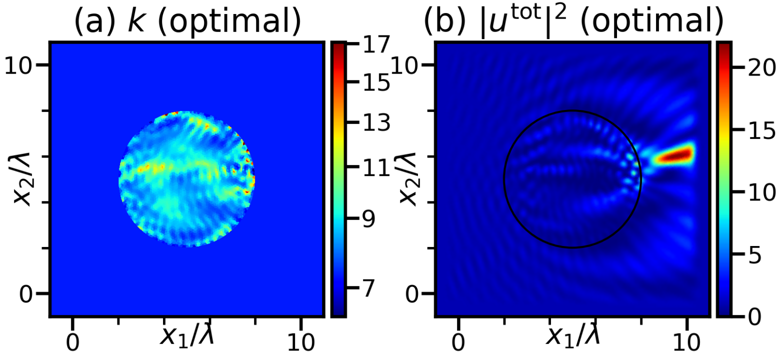
- M is the number of samples used in the SAA

The Lagrangian Formulation of the Objective

$$
\begin{aligned}
\mathcal{L}(\tau) =& \frac{1}{M} \sum_{m=1}^{M} \mathcal{Q}(\tau, \zeta_m) \\
&+ \beta_V \frac{1}{M} \sum_{m=1}^{M} \mathcal{Q}^2(\tau, \zeta_m) - \bar{\mathcal{Q}}^2 \\
&+ \beta_P P(\tau) \\
&+ \sum_{m=1}^{M} \left(a(u_m^{\text{sca}}, v_m; \tau, \zeta_m) - b(v_m) \right) . \qquad (7)
\end{aligned}
$$

- $a(u_m^{\text{sca}}, v_m; \tau, \zeta_m) = b(v_m)$, $\forall$ test function v_m is the weak form of the Helmholtz equation (v_m are also Lagrange multipliers)

Results: OUU using SAA



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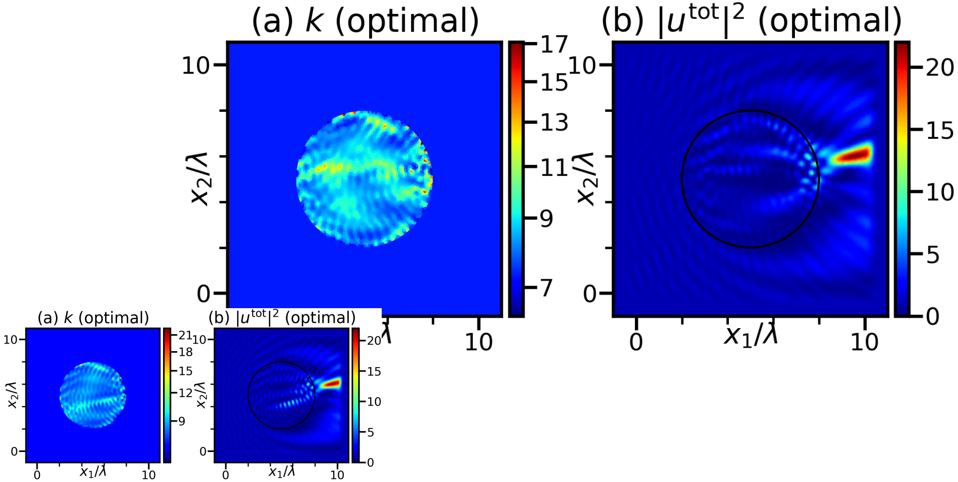
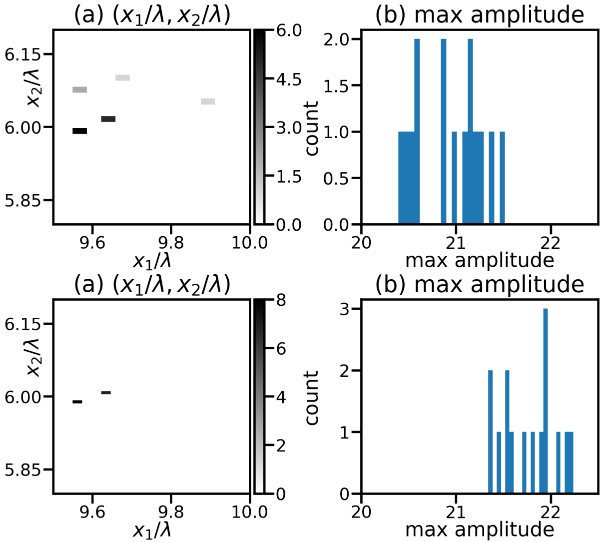


Results: Effect of Manufacturing Error

Deterministic

OUU



Effect of Manufacturing Error, Cont.

	x	y	max amp
mean (const.)	9.61	6.01	20.93
variance (const.)	0.0083	0.0015	0.112
mean (SAA)	9.59	5.99	21.76
variance (SAA)	0.0023	0.00015	0.078

Double the manufacturing error:

	x	y	max amp
mean (const.)	9.6	6.02	19.4
variance (const.)	0.02	0.005	1.27
mean (SAA)	9.61	6.01	21.76
variance (SAA)	0.008	0.0017	0.33

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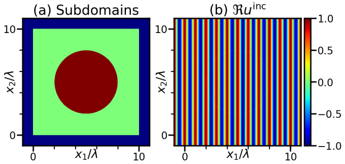
Practicality of manufacturing the result lens profile

- One way to build such profiles is 3D printing in liquid



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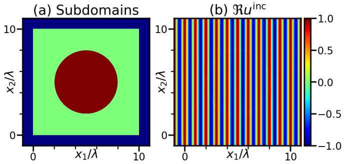

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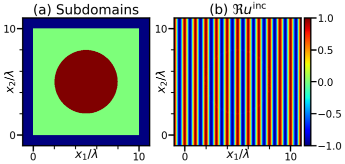

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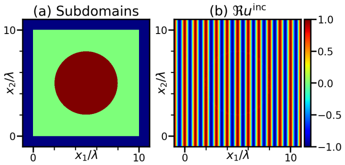

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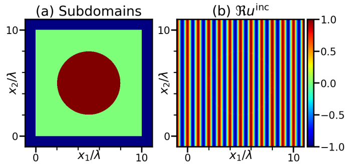
  - Sub-voxel-sized air bubbles
  - Material impurities
  - Deformations due to thermal expansion



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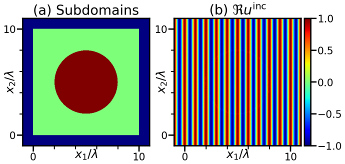
  - Deformations due to thermal expansion
- Can achieve higher relative resolution in e.g., microwave regimes (wavelength 1 cm)



Towards topology optimization of PNJ lens

In [Deng and Korvink, 2016]

- Enforce feature resolution by Helmholtz filter $\tau_f = H(\tau)$
- Projection to enforce binary material $P_\beta(\tau_f)$
- Here we apply the projection only directly on τ, $P_\beta(\tau)$

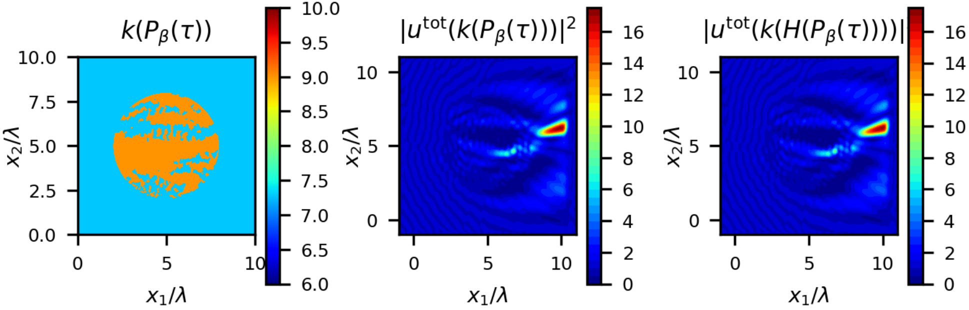
Threshold method (enforce binary material)

$$P_\beta(\tau) = \tau_p = \frac{\tanh(\beta\xi) + \tanh(\beta(\tau - \xi))}{\tanh(\beta\xi) + \tanh(\beta(1 - \xi))} \tag{8}$$

- $\xi \in [0, 1]$ and β are the threshold and projection parameters
- τ_p is the projected design

The optimization, revisited

- Objective: $\mathcal{Q}(u^{\text{tot}}(P_\beta(\tau)))$
- Optimization by continuation $\beta = 1, 5, 6, 6.5$
- Hard thresholding at last iteration
- $\max(|u^{\text{tot}}(K(P_\beta(\tau)))|^2) = 17.33$ and $\max(|u^{\text{tot}}(K(H(P_\beta(\tau))))|^2) = 17.22$



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- The obtained heterogeneous lens profile can achieve desired radial and angular shift in PNJ location and increase its amplitude
- Taking manufacturing uncertainty into account results in a non-trivial optimal profile that achieves more robust PNJ design
- Preliminary results using topology optimization techniques to obtain attainable lens profiles

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Thank you!