PCA: The Foundation for Metalens Design

White Paper

Version 1.0

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Executive Summary

This white paper presents the rationale behind the Periodic Cell Array (PCA) approximation as the intelligent foundation for metalens investigation.

Key insights:

- Metalenses operate on a fundamentally different principle than conventional optics: local wavefront control on a flat surface using sub-wavelength meta-atoms
- Evanescent coupling between neighboring meta-atoms introduces non-local effects that threaten the local design paradigm
- PCA restores local design while including crosstalk by substituting each meta-atom's neighborhood with an idealized array of identical neighboring meta-atoms
- Within this substituted structure, Maxwell's equations are solved rigorously using RCWA—PCA is not an approximation of the physics, but a structural substitution
- PCA enables first-order analysis: phase coverage, dispersion, aberrations, and polarization dependency
- Second-order effects (efficiency, higher orders, scattering from parameter jumps) are evaluated separately after PCA confirms feasibility

Why this matters for real-world metalenses:

- PCA enables the optical response of each meta-atom to be characterized independently of its neighbors
- This independent per-meta-atom characterization is the essential enabler for building **surrogate models** [1]
- Surrogate models make large-scale metalens design and simulation practical — the only way to handle millions of meta-atoms efficiently
- Without PCA, surrogate models would be impossible — neighbor couplings would force global, non-local characterization

For a detailed discussion of surrogate models and their role in fast design and simulation, see the companion white paper [1].

PCA for design is the only way to enable local design. Second-order analysis tools help to further evaluate performance.

Contents

1 The Local Design Principle on a Flat Surface

Conventional lenses control the wavefront through their three-dimensional shape—curved surfaces, varying thickness, and bulk material properties. The phase imparted at each point is determined by the optical path length through the glass, which varies smoothly across the aperture.

Metalenses offer a different approach: **local control of the wavefront on a flat surface**. At every position (x, y), a sub-wavelength meta-atom is chosen to impart a specific phase shift, and together they shape the wavefront. This local design principle—phase engineering on a planar substrate—is what makes metalenses different from conventional optics, and worth investigating for their potential in applications.

But here is the reality: because meta-atoms are sub-wavelength nanostructures, their electromagnetic interaction is not limited to propagating waves—**evanescent fields extend beyond each meta-atom and couple to neighboring meta-atoms**. These near-field interactions mean that the optical response at a given position depends not only on the local meta-atom geometry, but also on the geometries of neighboring meta-atoms. The response becomes non-local.

Taking into account these interdependencies between different meta-atoms rigorously would lead to an impossible situation:

- The optical response at every position depends on the entire surrounding neighborhood through evanescent coupling
- Changing one meta-atom geometry means re-evaluating the response across the entire lens
- Design becomes an iterative, global optimization problem
- The intuitive local design principle disappears

This is not just a matter of computational effort—it is a conceptual challenge. The beauty of metasurfaces lies in the local control of the optical response via each meta-atom. If we abandon this assumption, that beauty is lost. Moreover, a global optimization approach would require solving an enormous multi-dimensional problem (millions of meta-atoms, each with continuous geometric parameters), which is neither computationally feasible nor conceptually reasonable. Even with a fast solver, such an optimization would be a nightmare — with simulations taking hours or days per meta-atom type characterization, it is simply not a serious option for designing real-world metalenses.

2 PCA: The Enabler

The Periodic Cell Array (PCA) approximation makes a simple assumption: for the purpose of analyzing and designing a specific meta-atom, we replace its real, varying neighborhood with an idealized array of identical neighboring meta-atoms (see Fig. 1). This substitution is performed independently for each meta-atom position

across the lens.

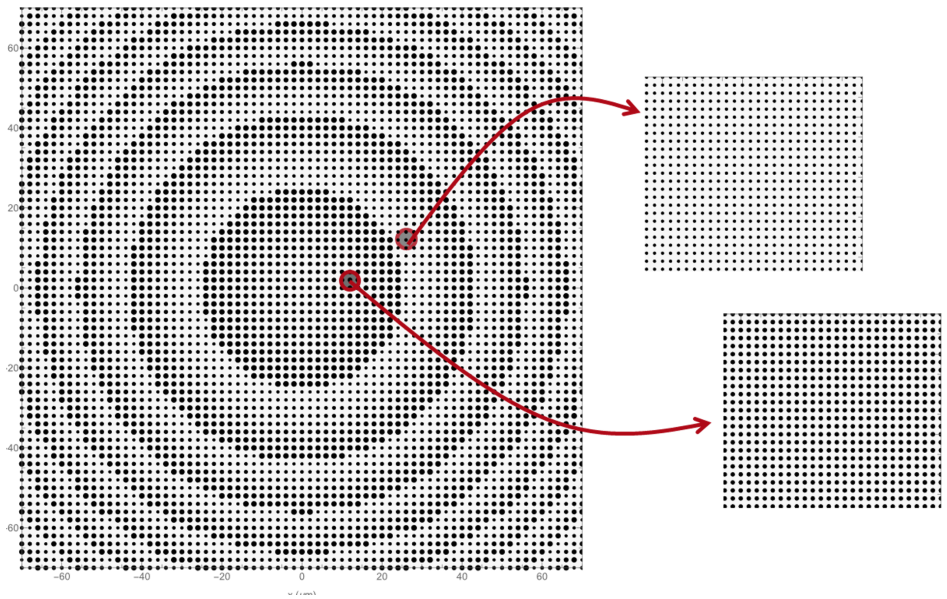

Figure 1: PCA substitution principle. A metalens with varying meta-atom geometries is shown. From selected meta-atom positions, arrows lead to their individual PCA substitutions: each is replaced by an infinite periodic array of meta-atoms identical to itself. The substitution is performed independently for every meta-atom position across the lens.

It is important to be precise about what this means:

- **PCA is not an approximation of Maxwell's equations.** Within the substituted structure, Maxwell's equations are solved rigorously using RCWA (Rigorous Coupled-Wave Analysis).
- **Crosstalk is included.** Unlike an isolated meta-atom model, PCA fully accounts for electromagnetic coupling within the array of identical neighbors. The calculated optical response for a given geometry includes interactions with its assumed-identical neighbors.
- **Yet design remains local.** Because the substitution assumes identical neighbors, the optical response depends only on the local geometry choice. This restores the local design principle while still capturing near-field coupling effects.

2.1 Enabling Local Design

The combination described above is what makes PCA a practical approach for design:

- **Crosstalk is included:** The optical response function is that of a meta-atom embedded in an environment of identical neighbors—including coupling effects
- **Design is local:** Despite including crosstalk, each meta-atom can still be

chosen independently based on its target phase

- **Intuition is preserved:** The relationship between geometry and optical response remains clear and direct
- **Investigation is enabled:** Engineers can explore what metalenses can do while maintaining the local design principle that makes metasurfaces attractive

2.2 Enabling Surrogate Models

The per-meta-atom characterization that PCA provides is not just about design convenience — it is the **essential enabler** for building surrogate models [1]. Because the optical response of each meta-atom can be characterized independently of its neighbors, we can:

- Characterize each meta-atom type once, across the full parameter space of geometries, wavelengths, angles, and polarizations
- Train neural network surrogate models from these characterizations
- Use these surrogate models for instant evaluation during design and simulation

Without PCA, surrogate models would be impossible. Neighbor couplings would force global, non-local characterization — the optical response of each meta-atom would depend on the configuration of its neighbors, making independent precomputation infeasible and simulation impractically slow.

PCA is therefore the **only path** to large-scale metalens design and simulation. It enables the surrogate models that make real-world metalenses — with millions of meta-atoms — tractable.

For a detailed discussion of surrogate model training, validation, and application, see the companion white paper [1].

PCA is not a compromise. It is an **enabling choice** that makes metalens design practical — including the essential physics of neighbor interactions while maintaining the local design paradigm on a flat surface.

3 PCA: The Right Tool

When you are investigating what metalenses can do for your application, PCA is the right tool.

It tells you:

- Can I achieve the phase profile I need on a flat surface?
- What dispersion behavior can I expect from my chosen geometries?
- How will the lens perform at different field angles?
- Is this worth pursuing further?

If PCA shows that metalenses cannot solve your problem — the phase coverage is

insufficient, the dispersion is too strong, the off-axis performance is unacceptable — then you have your answer. No amount of more rigorous modeling will turn a fundamentally unsuitable design into a working solution.

4 Design First — Then Evaluate Second-Order Effects

This is the practical workflow we recommend and our software supports:

1. **Design your metalens using PCA.** This gives you the local design principle, crosstalk included, and answers all first-order questions.
2. **Investigate first-order performance.** Phase coverage, dispersion, aberrations, polarization dependency — if these do not meet your requirements, the lens will not work. No second-order analysis will change that.
3. **If first-order results pass your judgement, then proceed to second-order evaluation.** Efficiency, higher orders, scattering — these determine how well the lens performs, not whether it works in principle.

Our software supports this workflow seamlessly. PCA handles design and first-order analysis. Tailored simulation models provide second-order evaluation without abandoning the local design principle.

If PCA shows promise — if the phase, dispersion, and aberration behavior align with your needs — then it is time to dig deeper. The PCA approximation assumes identical neighbors for each meta-atom. That assumption holds well for many regions of the lens, but not for all. Where it begins to weaken, second-order questions emerge.

You have completed the essential phase of your metalens journey: design and first-order characterization. Now it is time to ask:

- **Efficiency:** How much light actually reaches the focus? PCA provides an answer, but for smaller zones, it tends to overestimate.
- **Higher orders:** How much light goes into unwanted diffraction orders?
- **Scattering:** Do abrupt jumps between neighboring meta-atom parameters introduce scattering that could become a dealbreaker?

These are second-order questions. They do not affect whether the lens works in principle — PCA has already answered that. But they do affect whether the lens works well enough for your specific application. Answering them requires moving beyond the identical-neighbor assumption to simulation models that are tailored to provide answers on second-order effects — efficiency, higher orders, and scattering — while the design itself remains based on PCA.

This is not a redesign. The design remains based on PCA. Global optimization for design is not a viable option — it never was. Instead, these second-order tools provide further evaluation without abandoning the local design principle.

5 The Roughness Analogy

Consider conventional lens design. No one starts by modeling surface roughness. You begin with ideal surfaces, perfect anti-reflection coatings, and bulk materials. You establish that the lens can do what you need. Only then do you ask:

- What happens with realistic coatings?
- How sensitive is it to surface errors?
- What is the impact of manufacturing tolerances?

PCA plays the same role for metalenses. It is the **foundation** — including nearest-neighbor coupling effects, but assuming identical neighbors. It tells you whether the metalens can do the job with respect to first-order criteria — phase coverage, dispersion, aberrations, polarization dependency. If yes, then you can proceed to consider further details like efficiency, higher orders, and scattering.

6 Our Offering

We provide PCA-based solutions because they enable you to:

1. **Design with confidence:** PCA gives you a practical, local design method that includes crosstalk.
2. **Investigate first-order performance:** Phase coverage, dispersion, aberrations, polarization dependency — all answered efficiently.
3. **Decide systematically:** If the first-order results are promising, proceed. If not, stop. No wasted effort.
4. **Move to second-order evaluation only when needed:** Efficiency, higher orders, scattering — evaluated with tailored tools after PCA shows promise.

If the first-order results from PCA show that your metalens concept works, then — and only then — does it make sense to investigate second-order effects with specialized tools.

7 Conclusion

PCA is not a compromise. It is an intelligent foundation.

It is not an approximation of the physics — within the substituted structure, Maxwell's equations are solved rigorously using RCWA. It is a structural substitution that:

- **Includes crosstalk:** The calculated optical response captures coupling with identical neighbors
- **Preserves local design:** Each meta-atom can still be chosen independently
- **Enables flat-surface wavefront engineering:** The different approach of metaoptics becomes accessible for investigation

Moreover, PCA enables the optical response of each meta-atom to be characterized independently of its neighbors — the essential foundation for building surrogate models [1]. Surrogate models make large-scale metalenses with millions of meta-atoms tractable. Without PCA, surrogate models would be impossible.

Second-order evaluation has its place — after PCA confirms feasibility, when you need to quantify efficiency, higher orders, and scattering. But it does not replace PCA-based design. PCA remains the foundation.

The PCA Philosophy:

- **PCA for design:** The only way to enable local design on a flat surface
- **First-order analysis:** Functionality, aberrations, dispersion, polarization dependency
- **Enables surrogate models:** Independent per-meta-atom characterization for fast design and simulation [1]
- **Second-order evaluation:** Tailored tools to further evaluate performance

We provide the tools. You discover what metalens design works for you.

8 Outlook

If the first-order results from PCA show that your metalens concept is promising, then it is time to investigate second-order effects — efficiency, higher orders, scattering — with tailored simulation models.

8.1 From PCA to Metagrating Analysis

As we move toward the outer zones of a metalens, the neighborhood of a meta-atom becomes less like an array of identical neighbors and more like a grating — periodic in the radial direction with gradually varying parameters across zones. For evaluating second-order effects in these regions, a different structural substitution becomes appropriate: the Local Metagrating Approximation (LMGA).

8.2 Efficiency Predictions: PCA vs. LMGA

The choice of substitution affects efficiency predictions, particularly as zone periods become smaller. Figure 3 shows how LMGA efficiencies deviate from PCA predictions for decreasing periods. Note that the example in the table does not directly show a metalens, but gratings with periods corresponding to the zone widths of a metalens — and by that to the associated local numerical aperture (NA).

First, recall how both methods relate to RCWA:

- **PCA** applies RCWA to a subwavelength periodic cell array — an infinite array of identical meta-atoms. This is used both for **design** (selecting meta-atom geometries based on phase) and for first-order **efficiency evaluation**.

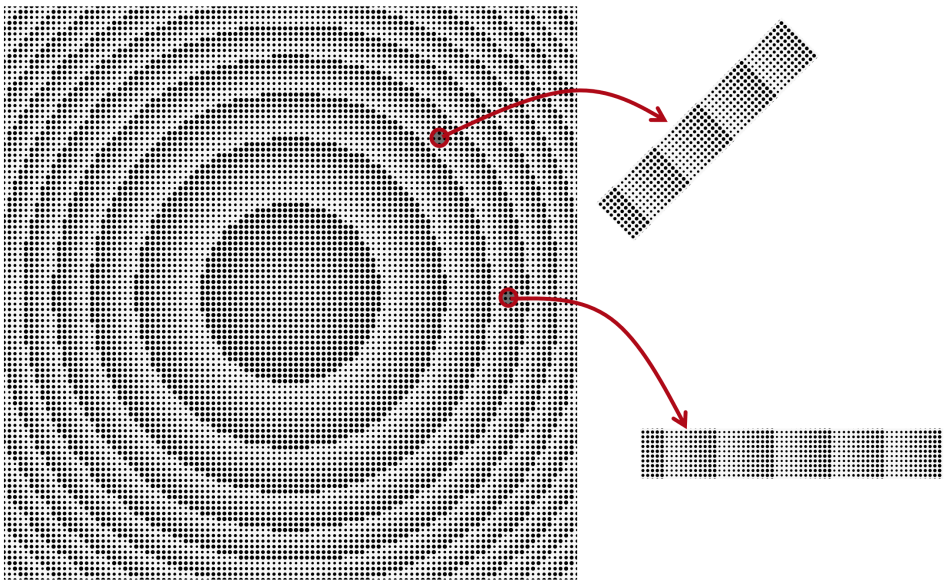

Figure 2: LMGA substitution principle for second-order evaluation. From selected meta-atom positions in the outer zones of a metalens, arrows point to their substitution as local metagratings. The period of each metagrating corresponds to the local zone width, providing a different representation than identical-neighbor PCA — tailored for evaluating efficiency and higher orders. The design itself remains based on PCA.

- **LMGA** applies RCWA to a local metagrating of the type illustrated in Fig. 2 — a periodic structure where the period corresponds to the local zone width. The metagrating itself is designed via PCA (its meta-atoms come from the PCA design), but its efficiency is evaluated by applying RCWA to the entire grating, not to individual cell arrays.

In other words: PCA provides the design and a first estimate of efficiency. LMGA then evaluates the same design — without changing it — by applying RCWA to the actual local grating structure.

As shown in Fig. 3, PCA tends to overestimate efficiency as periods become smaller (zones become narrower). LMGA provides a different evaluation — again, for **assessment**, not for redesign.

8.3 Planned Capabilities

We will release a metagrating twin for systematic second-order evaluation in a future version. For a final error budget analysis, we are preparing a tool that enables the evaluation of PCA-predicted meta-atom optical response values at selected positions across the metalens.

With both steps, second-order effects can be evaluated before final prototyping — without abandoning the local design principle.

Period/ Lambda	NA of Lens	Efficiency of Desired Order		Reflected light		Transmitted orders (LMGA)
		PCA	LMGA	PCA	LMGA	
10.6	0.094	95.9 %	94.4 %	4.1 %	3.8 %	1.8 %
5.3	0.189	95.9 %	92.6 %	4.1 %	4.4 %	3 %
3.2	0.313	95.9 %	86.7 %	4.1 %	8.5 %	4.8 %
2.9	0.345	95.9 %	87.6 %	4.1 %	7.5 %	4.9 %
2.1	0.476	95.9 %	82.2 %	4.1 %	12.3 %	5.5 %
1.3	0.769	95.9 %	76.6 %	4.1 %	19.6 %	3.8 %

Figure 3: Comparison of efficiency predictions: PCA (cell array with identical neighbors) vs. LMGA (local metagrating) for decreasing periods. The example shows gratings with periods corresponding to zone widths of a metalens — and by that to the associated NA. The grating is designed via PCA; LMGA evaluates its efficiency by applying RCWA to the entire grating. PCA tends to overestimate efficiency as the period decreases (higher NA). LMGA provides a different evaluation — for **assessment**, not for redesign.

Key message:

- PCA for design is the only way to enable local design.
- PCA enables first-order analysis of functionality, aberrations, dispersion, and polarization dependency.
- PCA enables surrogate models [1] — independent per-meta-atom characterization for fast design and simulation.
- Second-order evaluation tools — with a different emphasis — help to further evaluate performance.

A Document Version History

Version	Date	Changes
1.0	April 2026	Initial release with figures, tables, and outlook

References

[1] Frank Wyrowski. *Surrogate Modeling: Enabling Practical Metalens Design and Simulation*. White Paper WP-META-SURROGATE. LightTrans International GmbH, 2026. link.