Optimization of Two-Lens Coupling Systems for VUV Flashlamp to Fiber Applications Using Ray Tracing and Multi-Algorithm Comparison

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Abstract

A comprehensive ray tracing methodology is presented for optimizing two-lens plano-convex optical systems designed to couple vacuum ultraviolet (VUV) light from the Hamamatsu L7685 60W xenon flash lamp into optical fibers for liquid argon purity monitoring applications. Operating at 200 nm wavelength, the system addresses the challenge of efficiently collecting light from a 3 mm diameter arc source with a 66° divergence angle and coupling it into a 1 mm core fiber with 0.22 numerical aperture. A stratified ray tracing approach incorporating full geometric optics and atmospheric absorption is employed. Six optimization algorithms—grid search, Powell's method, differential evolution, Nelder-Mead simplex, dual annealing, and Bayesian optimization—are implemented in a modular framework and systematically compared on the plano-convex optical design problem. Deterministic ray tracing evaluates coupling efficiency by propagating 1000 rays through the optical system and testing acceptance at the fiber face. Atmospheric absorption by O_2, N_2, and H_2O is modeled using empirical parameterizations. The best configurations achieve coupling efficiencies of 0.19–0.24 in air and 0.24–0.27 in argon atmosphere, representing an $\sim$8% improvement due to eliminated O_2 absorption at 200 nm, with compact system lengths of 35–41 mm for optimized configurations. Powell's method emerges as the most effective algorithm for routine optimization, achieving rapid convergence (1–2 seconds per lens pair) while finding high-quality solutions. Differential evolution provides thorough global exploration when needed (10–17 seconds per lens pair). Comparison of air and argon propagation media reveals the $\sim$8% coupling improvement in argon due to eliminated atmospheric absorption, though air remains practical for applications tolerating modest efficiency reduction. Wavelength analysis across 150–300 nm reveals peak performance in the 220–260 nm range, with severe degradation below 180 nm in air where coupling drops nearly to zero. The multi-objective optimization framework successfully balances coupling efficiency and system compactness through a tunable weighted objective function. This work provides both a practical computational tool for VUV fiber coupling design and methodological insights into optimization strategy selection for non-convex optical design problems.

1 Introduction

Efficient coupling of vacuum ultraviolet light from incoherent sources into optical fibers presents significant challenges due to the inherent divergence of arc lamp sources and the limited acceptance angles of fibers [1]. The Hamamatsu L7685 60W xenon flash lamp provides a compact broadband source (190–2000 nm) suitable for liquid argon purity monitoring applications in the VUV range. This work focuses on optimizing coupling at the design wavelength of 200 nm, where fiber-optic delivery enables remote sensing and flexible optical system configurations in cryogenic environments.

The design of compact coupling optics requires balancing multiple objectives: maximizing coupling efficiency, minimizing physical length, and maintaining practical manufacturability with commercially available optical components. Traditional lens design approaches often rely on paraxial approximations or specialized optical design software [2]. However, the large numerical aperture and wide divergence angles in VUV flashlamp systems necessitate full ray tracing to accurately predict system performance.

In this work, a stratified ray tracing framework is developed that incorporates realistic source geometry, lens specifications, fiber acceptance criteria, and atmospheric absorption effects (O_2, N_2, and H_2O). The design problem is formulated as a multi-objective optimization task, and six distinct optimization algorithms are systematically compared to identify lens positioning that maximizes performance. This approach provides both a practical design tool and insights into the efficacy of various optimization strategies for optical systems with complex, non-convex objective functions characterized by multiple local optima and discrete ray-counting mechanics that preclude analytical gradient computation.

2 System Description

2.1 Optical Configuration

The optical system comprises a Hamamatsu L7685 60W xenon flash lamp [3], a Single Crystal Sapphire Glass protective window, two fused silica plano-convex lenses, and a multi-mode optical fiber [4] arranged along a common optical axis. The lamp emits broadband radiation (190–2000 nm) from a compact 3.0 mm diameter arc; this work analyzes coupling performance at $\lambda = 150$–300 nm. The Single Crystal Sapphire Glass window (14.3 mm diameter) positioned 8.7 mm from the arc protects the source while allowing VUV transmission. The two-lens relay system is positioned after the window to collect and refocus the divergent light into the fiber.

2.2 Source Characteristics

The xenon arc source exhibits a spatially extended emission profile with angular divergence that increases radially from the arc center. The source is modeled as emitting rays from a circular disk of radius $r_{\text{arc}} = 1.5$ mm with angular distribution characterized by a maximum half-angle $\theta_{\max} = 33°$ at the window edge. This coherent beam model assumes that rays originating at radius r from the arc center propagate with half-angle $\theta(r) = \theta_{\max} \cdot r/r_{\text{arc}}$, representing the geometric constraint imposed by the window aperture.

2.3 Fiber Specifications

The target optical fiber features a 1.0 mm core diameter with numerical aperture NA = 0.22, corresponding to an acceptance half-angle $\theta_{\text{accept}} = \sin^{-1}(\text{NA}) = 12.4°$ in air. Successful coupling requires that incident rays satisfy both spatial (impinge within the core area) and angular (arrive within the acceptance cone) criteria simultaneously.

2.4 Lens Properties

All lenses are fabricated from UV-grade fused silica with refractive index $n = 1.578$ at 200 nm, calculated using the Sellmeier dispersion formula [5]. Plano-convex geometry is selected for its favorable aberration characteristics and commercial availability. Lenses are oriented with the curved surface facing the source to minimize spherical aberration. Specifications including focal length f, radius of curvature R, center thickness t_c, edge thickness t_e, and clear aperture diameter are drawn from manufacturer catalogs [6, 7].

3 Computational Methods

3.1 Stratified Ray Sampling

A stratified sampling approach is employed to efficiently sample the phase space of rays emitted by the extended source. For each simulation, $N = 1000$ to 2000 rays are generated with origins uniformly distributed over the arc area and directions following the prescribed angular distribution.

Radial positions are sampled using inverse transform sampling to ensure uniform spatial distribution:

$$r_i = \sqrt{U_i} \cdot r_{\text{arc}}, \quad U_i \sim \mathcal{U}(0,1) \tag{1}$$

$$\phi_i = \frac{2\pi i}{N} \tag{2}$$

where $\mathcal{U}(0,1)$ denotes the uniform distribution. Azimuthal angles ϕ_i are uniformly spaced to provide comprehensive angular coverage. The Cartesian coordinates of source points are:

$$\mathbf{o}_i = (r_i \cos\phi_i,\, r_i \sin\phi_i,\, 0) \tag{3}$$

The ray propagation half-angle scales linearly with radial position:

$$\theta_i = \theta_{\max} \cdot \frac{r_i}{r_{\text{arc}}} \tag{4}$$

resulting in direction vectors:

$$\mathbf{d}_i = (\sin\theta_i \cos\phi_i,\, \sin\theta_i \sin\phi_i,\, \cos\theta_i) \tag{5}$$

All direction vectors are normalized to unit length.

3.2 Geometric Ray Tracing

Ray propagation through the optical system is computed using vector-based geometric optics without paraxial approximations [8]. This approach accurately accounts for large ray angles, finite apertures, and aberrations.

3.2.1 Ray-Surface Intersection

For a spherical surface of radius R centered at $\mathbf{c}$, the intersection of ray $\mathbf{p}(t) = \mathbf{o} + t\mathbf{d}$ is found by solving:

$$\|\mathbf{o} + t\mathbf{d} - \mathbf{c}\|^2 = R^2 \tag{6}$$

Expanding yields the quadratic equation:

$$a = 1 \tag{7}$$

$$b = 2(\mathbf{o} - \mathbf{c}) \cdot \mathbf{d} \tag{8}$$

$$c = \|\mathbf{o} - \mathbf{c}\|^2 - R^2 \tag{9}$$

$$\Delta = b^2 - 4c \tag{10}$$

The nearest positive intersection occurs at:

$$t = \frac{-b - \sqrt{\Delta}}{2}, \quad \Delta \geq 0 \tag{11}$$

Rays missing the surface ($\Delta < 0$) or blocked by the aperture ($\sqrt{p_x^2 + p_y^2} > r_{\text{ap}}$) are rejected.

3.2.2 Vector Refraction

At each refractive interface, Snell's law is applied in vector form. For incident ray $\mathbf{d}_{\text{in}}$, surface normal $\mathbf{n}$ (pointing into the incident medium), and refractive indices n_1 and n_2:

$$\eta = \frac{n_1}{n_2} \tag{12}$$

$$\cos\theta_i = -\mathbf{n} \cdot \mathbf{d}_{\text{in}} \tag{13}$$

$$k = 1 - \eta^2(1 - \cos^2\theta_i) \tag{14}$$

Total internal reflection occurs when $k < 0$. Otherwise, the refracted ray is:

$$\mathbf{d}_{\text{out}} = \eta\mathbf{d}_{\text{in}} + (\eta\cos\theta_i - \sqrt{k})\mathbf{n} \tag{15}$$

For the spherical front surface, the outward normal is $\mathbf{n} = (\mathbf{p} - \mathbf{c})/R$. For the planar back surface, $\mathbf{n} = (0, 0, -1)$.

3.2.3 Lens Propagation

Within each lens, the ray propagates a distance determined by the local lens thickness. For a plano-convex lens with center thickness t_c and edge thickness t_e, the thickness at radial position r is:

$$t_{\text{local}}(r) = t_c - (t_c - t_e) \cdot \frac{r}{r_{\text{ap}}} \tag{16}$$

The exit point on the back surface is:

$$\mathbf{o}_{\text{back}} = \mathbf{p}_{\text{front}} + \frac{t_{\text{local}}}{|d_z|}\mathbf{d}_{\text{refracted}} \tag{17}$$

3.3 Fiber Coupling Analysis

After traversing both lenses, rays propagate to the fiber face located at $z = z_{\text{fiber}}$. The intersection point is computed as:

$$\mathbf{p}_{\text{fiber}} = \mathbf{o}_2 + \frac{z_{\text{fiber}} - o_{2z}}{d_{2z}}\mathbf{d}_2 \tag{18}$$

where $\mathbf{o}_2$ and $\mathbf{d}_2$ are the ray origin and direction after the second lens.

A ray successfully couples into the fiber if:

1. *Spatial criterion*: $\sqrt{p_x^2 + p_y^2} \leq r_{\text{core}} = 0.5$ mm
2. *Angular criterion*: $\theta = \arccos\big(|d_{2z}|/\|\mathbf{d}_2\|\big) \leq \theta_{\text{accept}} = 12.4°$

The coupling efficiency is:

$$\eta_{\text{coupling}} = \frac{N_{\text{accepted}}}{N_{\text{total}}} \tag{19}$$

4 Optimization Framework

4.1 Problem Formulation

The optical design task is formulated as a constrained multi-objective optimization problem. Given a pair of lenses with fixed optical properties (focal lengths f_1 and f_2, radii of curvature, thicknesses, and apertures), the optimal axial positions are sought that maximize coupling efficiency while minimizing overall system length.

4.1.1 Design Variables

The optimization space comprises three continuous parameters:

- z_1: axial position of the first lens vertex (mm)
- z_2: axial position of the second lens vertex (mm)
- z_{fiber}: axial position of the fiber face (mm)

Physical constraints ensure feasible configurations:

$$z_1 \geq z_{\text{window}} + \Delta z_{\text{min}} = 9.7 \text{ mm} \tag{20}$$

$$z_2 > z_1 + 0.1 \text{ mm} \tag{21}$$

$$z_{\text{fiber}} \approx z_2 + f_2 \tag{22}$$

where the fiber position is typically placed one focal length beyond the second lens as a starting approximation.

4.1.2 Objective Function

A weighted-sum scalarization is employed to combine coupling efficiency maximization and length minimization:

$$\min_{z_1, z_2} f(z_1, z_2) = \alpha(1 - \eta_{\text{coupling}}) + (1 - \alpha)\frac{z_{\text{fiber}}}{L_{\text{norm}}} \tag{23}$$

where $\alpha \in [0, 1]$ is the preference weight (default $\alpha = 0.7$ prioritizes coupling), and $L_{\text{norm}} = 80$ mm is a normalization length. This formulation converts both objectives to minimization with comparable scales.

Each evaluation of $f(z_1, z_2)$ requires complete ray tracing of N rays through the system, making the objective function computationally expensive and non-differentiable due to discrete ray counting and aperture clipping.

4.2 Optimization Algorithms

Six optimization methods are implemented and compared, representing different algorithmic paradigms: exhaustive search, local gradient-free methods, and global stochastic approaches.

4.2.1 Grid Search

An exhaustive two-stage search, implemented from scratch, establishes a performance baseline. In the coarse stage, a 7×7 grid samples the parameter space with bounds determined by lens focal lengths:

$$z_1 \in [9.7, \max(14.7, 1.5f_1)] \tag{24}$$

$$z_2 \in [z_1 + 0.5f_2, z_1 + 2.5f_2] \tag{25}$$

The best coarse solution undergoes local refinement via a 9×9 grid spanning $\pm 2\Delta$ around the coarse optimum, where Δ is the coarse grid spacing. Total evaluations: 130 per lens pair.
Implementation: `scripts/optimization/grid_search.py`. Uses 500 rays per evaluation to balance accuracy and speed. Fiber position is fixed at $z_{\text{fiber}} = z_2 + f_2$ for each (z_1, z_2) pair.

4.2.2 Powell's Method

Powell's conjugate direction method [9] performs derivative-free local optimization by iteratively minimizing along coordinate axes and constructed conjugate directions. The algorithm is particularly effective for smooth, unimodal functions.
Implementation uses SciPy's `optimize.minimize` with method `'Powell'` [10]. Parameters: 200 maximum iterations, position tolerance $\Delta x = 0.01$ mm, function tolerance $\Delta f = 0.001$. Initial guess: $z_1^{(0)} = \max(9.7, 0.8f_1)$, $z_2^{(0)} = z_1^{(0)} + 1.2f_2$. Uses 1000 rays per evaluation for higher precision than grid search.
Module: `scripts/optimization/powell.py`. Typically converges in 30–50 function evaluations.

4.2.3 Nelder-Mead Simplex

The Nelder-Mead algorithm [11] maintains a simplex of $n + 1$ points in n-dimensional space, updating via geometric transformations (reflection, expansion, contraction, shrinkage). It is robust to function noise and requires no derivatives.
Implementation uses SciPy's `optimize.minimize` with method `'Nelder-Mead'` [10]. Parameters: 200 maximum iterations, position tolerance 0.01 mm, function tolerance 0.001. Same initialization as Powell's method. Uses 1000 rays per evaluation.
Module: `scripts/optimization/nelder_mead.py`. Fastest local method, typically converging in 20–40 evaluations.

4.2.4 Differential Evolution

Differential evolution [12] is a population-based global optimizer using evolutionary strategies. At each generation, trial vectors are created via:

$$\mathbf{x}_{\text{trial}} = \mathbf{x}_r + F(\mathbf{x}_a - \mathbf{x}_b) \tag{26}$$

where $\mathbf{x}_r$, $\mathbf{x}_a$, $\mathbf{x}_b$ are randomly selected population members and F is the mutation factor. Trial vectors compete with current population members via greedy selection.
Implementation uses SciPy's `optimize.differential_evolution` [10]. Parameters: population size 10, maximum 50 iterations, tolerance 0.001. Bounds as specified for grid search. Uses 1000 rays per evaluation.
Module: `scripts/optimization/differential_evolution.py`. Provides thorough global exploration when robustness is critical. Typical evaluations: 60–100.

4.2.5 Dual Annealing

Dual annealing [13, 14] combines classical simulated annealing with local search to escape local minima. The algorithm accepts worse solutions probabilistically according to the Boltzmann criterion:

$$P_{\text{accept}} = \exp\left(-\frac{\Delta f}{k_B T}\right) \tag{27}$$

where T decreases according to an adaptive cooling schedule.
Implementation uses SciPy's `optimize.dual_annealing` [10]. Parameters: 300 maximum iterations, same bounds as differential evolution. Uses 1000 rays per evaluation. The algorithm alternates between global exploration (simulated annealing) and local refinement (L-BFGS-B).
Module: `scripts/optimization/dual_annealing.py`. Effective for highly multi-modal landscapes. Typical evaluations: 80–120.

4.2.6 Bayesian Optimization

Bayesian optimization [15, 16] builds a Gaussian process (GP) surrogate model of the objective function and selects evaluation points by maximizing an acquisition function, typically expected improvement (EI):

$$\text{EI}(\mathbf{x}) = \mathbb{E}[\max(f_{\text{best}} - f(\mathbf{x}), 0)] \tag{28}$$

This approach is sample-efficient, making it suitable for expensive objectives. The GP provides uncertainty estimates that guide exploration-exploitation trade-offs.
Implementation uses scikit-optimize's `gp_minimize` [17]. Parameters: 50 total function evaluations (reduced from original 100 for computational efficiency), 10 initial random samples, remaining samples via EI maximization. Uses 1000 rays

per evaluation. Requires additional package: `pip install scikit-optimize`.
Module: `scripts/optimization/bayesian.py`. Best suited when function evaluations are extremely expensive or when uncertainty quantification is desired.

5 Material Properties

The refractive index of fused silica at VUV wavelengths is calculated using the Sellmeier dispersion equation [5]:

$$n^2(\lambda) = 1 + \sum_{i=1}^{3} \frac{B_i \lambda^2}{\lambda^2 - C_i} \tag{29}$$

with Malitson coefficients:

$$\begin{aligned} B_1 &= 0.6961663, \quad C_1 = (0.0684043)^2 \\ B_2 &= 0.4079426, \quad C_2 = (0.1162414)^2 \\ B_3 &= 0.8974794, \quad C_3 = (9.896161)^2 \end{aligned}$$

where wavelength λ is expressed in micrometers. At the operating wavelength $\lambda = 0.2$ μm (200 nm), this yields $n = 1.578$.

6 Atmospheric Attenuation

At VUV wavelengths, molecular oxygen (O_2) exhibits strong absorption that significantly attenuates light propagation through air. This effect must be accounted for to accurately predict coupling efficiency in practical systems.

6.1 Beer-Lambert Absorption

The transmission of light through an absorbing medium follows the Beer-Lambert law:

$$T = \exp(-\alpha d) \tag{30}$$

where T is the fractional transmission, α is the wavelength-dependent attenuation coefficient (mm^{-1}), and d is the propagation distance (mm). The attenuation coefficient for a multi-component gas mixture is:

$$\alpha(\lambda) = \sum_i \sigma_i(\lambda) n_i \tag{31}$$

where $\sigma_i(\lambda)$ and n_i denote the absorption cross-section and number density of species i, in units of cm^2 and molecules/cm^3, respectively.

6.2 O_2 Absorption Cross-Section

At 200 nm, oxygen absorption dominates atmospheric attenuation. The cross-section is computed using the Minschwaner parameterization [18], valid for 175–242 nm:

$$\log_{10} \sigma_{O_2}(\lambda) = a_0 + a_1\lambda + a_2\lambda^2 + a_3\lambda^3 + a_4\lambda^4 + a_5\lambda^5 - 16 \tag{32}$$

with coefficients:

$$\begin{aligned} a_0 &= -4.4011 \times 10^1, \quad a_1 = 6.2067 \times 10^{-1} \\ a_2 &= -3.5668 \times 10^{-3}, \quad a_3 = 9.5745 \times 10^{-6} \\ a_4 &= -1.2775 \times 10^{-8}, \quad a_5 = 6.6574 \times 10^{-12} \end{aligned}$$

where λ is in nanometers and σ is in cm^2. At 200 nm, this yields $\sigma_{O_2} = 1.15 \times 10^{-20}$ cm^2.

6.3 Number Density Calculation

Number densities are computed from the ideal gas law:

$$n = \frac{P}{k_B T} \tag{33}$$

where P is pressure, T is temperature, and $k_B = 1.381 \times 10^{-23}$ J/K is Boltzmann's constant. At standard conditions ($P = 1$ atm, $T = 293$ K), the total number density is $n_{\text{total}} = 2.50 \times 10^{19}$ molecules/cm^3.
For dry air composition:

$$n_{O_2} = 0.21 \times n_{\text{total}} = 5.25 \times 10^{18} \text{ cm}^{-3} \tag{34}$$

$$n_{N_2} = 0.78 \times n_{\text{total}} = 1.95 \times 10^{19} \text{ cm}^{-3} \tag{35}$$

N_2 absorption is negligible above 100 nm. Water vapor (typically $\sim$1% by volume) contributes minor additional absorption.

6.4 Attenuation Implementation

The attenuation coefficient for air at 200 nm is:

$$\alpha_{\text{air}} = \sigma_{O_2} n_{O_2} \approx 0.060 \text{ mm}^{-1} \tag{36}$$

Each ray's intensity is attenuated according to its cumulative path length d_{total} through air:

$$I_{\text{fiber}} = I_0 \exp(-\alpha_{\text{air}} d_{\text{total}}) \tag{37}$$

where d_{total} includes propagation from arc to window, inter-lens distances, and lens-to-fiber distance. For typical system lengths of 30–100 mm, transmission ranges from 16% to 0.25%, representing substantial loss.
This absorption model is implemented in `scripts/calcs.py` using cross-section data from `scripts/hitran_data.py`.

7 Model Assumptions and Validity

The ray tracing model incorporates several simplifying assumptions:

1. *Geometric optics regime*: The wavelength ($\lambda = 200$ nm) is negligible compared to all physical dimensions (apertures $\sim$ 1-25 mm), validating the ray approximation and neglecting diffraction effects.

2. *Simplified angular distribution*: The angular distribution is deterministic with respect to radial position. The actual Hamamatsu L7685 lamp contains an internal reflector that modifies the emission pattern; this model represents a simplified geometric approximation of the effective beam profile at the window.

3. *Perfect optical surfaces*: Surface roughness, figure errors, and manufacturing imperfections are neglected. Real VUV optics may deviate from ideal spherical and planar surfaces.

4. *Atmospheric absorption included; surface losses neglected*: Molecular absorption (primarily O_2 at 200 nm) is modeled using the Beer-Lambert law with Minschwaner cross-sections. However, Fresnel reflections at each air-glass interface (approximately 4-5% per surface at 200 nm, totaling ∼20% for 4 surfaces) and bulk absorption in fused silica are not included. Reported coupling efficiencies represent geometric coupling attenuated only by atmospheric absorption.

5. *Monochromatic light*: Chromatic aberration is absent. Real flashlamp spectra span broad wavelength ranges.

6. *Perfect alignment*: Lens decentration, tilt, and fiber misalignment errors are assumed zero. Practical systems require careful alignment procedures.

7. *Uniform fiber acceptance*: The numerical aperture is assumed constant across the core. Variations due to fiber manufacturing tolerances are ignored.

These assumptions are appropriate for design-stage performance prediction. The inclusion of atmospheric absorption provides more realistic coupling estimates for practical air-filled systems. Experimental validation would additionally require accounting for Fresnel losses and alignment tolerances.

8 Results

8.1 Implementation Architecture

The optimization framework is implemented as a modular Python system with separate modules for each algorithm located in `scripts/optimization/`. A unified runner interface (`optimization_runner.py`) provides consistent access to all methods through a common API. The command-line interface (`raytrace.py`) provides six operational modes:

- `particular`: Optimize a specific lens pair with chosen algorithm
- `compare`: Evaluate all six algorithms on a single lens pair
- `select`: Optimize 3,876 strategically chosen lens combinations (68 L1 candidates × 57 L2 candidates)
- `select-ext`: Extended selection mode with refined lens candidate filters and coupling thresholds
- `combine`: Exhaustive optimization of all 24,336 lens combinations (156 × 156)
- `analyze`: Re-optimize previously identified high-coupling configurations with all methods
- `wavelength-analyze`: Evaluate coupling efficiency across wavelength ranges for specific configurations

Additional features include automatic checkpoint/resume for interrupted batch runs, comprehensive logging with timestamps, CSV output for all results, and rich visualization capabilities (ray trace diagrams, spot diagrams, wavelength-dependent coupling plots). The modular architecture enables straightforward addition of new algorithms or objective functions.

8.2 Performance Comparison

Table 1 presents a systematic comparison of all six optimization methods applied to the best-performing lens pair (36-681 + 36-681) at 200 nm. Each method was evaluated on coupling efficiency achieved and total system length in both air and argon propagation media. All simulations use 1000 rays and the default weighted objective ($\alpha = 0.7$).

Table 1: Optimization Algorithm Performance Comparison at 200 nm (lens pair: 36-681 + 36-681)

Method	**Air η**	**Air L (mm)**	**Argon η**	**Argon L (mm)**
Grid Search	0.201	38.2	0.231	38.2
Powell	**0.238**	35.0	**0.248**	34.9
Nelder-Mead	0.209	35.3	0.004	31.8
Diff. Evol.	0.222	34.9	0.248	34.9
Dual Anneal.	0.223	35.0	0.234	34.9
Bayesian	0.207	40.0	0.227	40.0

Powell's method emerges as the recommended default for routine optimization, completing in 1–2 seconds per lens pair with reliable convergence. Nelder-Mead provides comparable speed as an alternative simplex-based approach. For the most thorough global search, differential evolution requires 10–17 seconds per pair but explores the parameter space more exhaustively, making it valuable for final verification of critical designs or difficult optimization landscapes. Bayesian optimization (20–22s) and dual annealing (40–51s) offer additional global search capabilities but at higher computational cost. Grid search (2–3s with default 7×7 grid) provides systematic baseline comparisons.

However, Nelder-Mead occasionally fails on certain lens combinations, returning physically invalid configurations with near-zero coupling. This robustness issue makes Powell's method the safer choice for batch processing of large lens catalogs, where individual monitoring of each optimization is impractical.

Key findings:

- *Powell's method* achieves the highest coupling in air (0.238) and ties with differential evolution in argon (0.248), demonstrating that local optimization can be highly effective with appropriate initialization. Convergence is rapid (∼1–2 s per lens pair), making it the recommended default for routine use.
- *Differential evolution* provides robust performance across both media (air: 0.222, argon: 0.248), though not always achieving the absolute best solution. It provides 3–4× speedup over grid search (typical: 10–17 s vs 38 s per lens pair) with good global exploration, making it valuable when thoroughness is prioritized over speed.
- *Nelder-Mead* converges fastest (0.4–2.0 s) but shows critical robustness issues. It fails catastrophically in argon for this lens pair ($\eta = 0.004$), highlighting the risk of poor local optima and making it unsuitable for unmonitored batch processing.
- *Grid search* provides a reliable baseline by exhaustively sampling configurations, though computational cost scales poorly for finer resolution or higher-dimensional searches.
- *Dual annealing* and *Bayesian optimization* find moderate solutions but with greater variability and computational overhead. Bayesian requires the additional `scikit-optimize` dependency.
- *Medium comparison:* Argon provides modest coupling improvement (4.2% for this lens pair) due to reduced O_2 absorption. Optimal system geometries remain nearly identical across media ($\Delta L < 0.5$ mm for successful methods).

8.3 Multi-Objective Optimization Results

The weighted objective function with tunable parameter α enables exploration of the coupling-compactness trade-off. Figure 2 (not shown) illustrates the Pareto frontier for selected lens pairs.

For the best lens combination 36-681 + 36-681 at 200 nm with $\alpha = 0.7$ (balanced, default):

Air propagation:

- Best method (Powell): $\eta = 0.238$, $L = 35.0$ mm
- Differential evolution: $\eta = 0.222$, $L = 34.9$ mm
- Dual annealing: $\eta = 0.223$, $L = 35.0$ mm

Argon propagation:

- Best methods (Powell, Diff. Evol.): $\eta = 0.248$, $L = 34.9$ mm
- Dual annealing: $\eta = 0.234$, $L = 34.9$ mm
- Grid search: $\eta = 0.231$, $L = 38.2$ mm

This lens pair achieves excellent compactness ($L \approx 35$ mm) without significant coupling degradation. The optimal geometry places the first lens approximately 10 mm from the source window and the second lens 13 mm downstream, resulting in a total system length of 35 mm to the fiber face. This configuration effectively balances beam collection from the divergent source with refocusing into the fiber acceptance cone.

The choice of optimization method affects performance: Powell's method finds better local optima in air when properly initialized, while differential evolution provides more robust global exploration. For this lens pair, system length remains remarkably consistent across methods ($L = 34.9$–35.3 mm for successful optimizations), indicating a well-defined optimal geometry.

Other lens combinations require longer focal lengths and achieve similar coupling at the cost of increased system length (38–47 mm).

8.4 Lens Selection Analysis

Analysis of high-performing configurations across multiple lens pair evaluations at 200 nm reveals consistent design principles:

Air propagation at 200 nm (best compact configurations using Powell's method):

- *Best overall*: 36-681 + 36-681 achieved $\eta = 0.238$ with $L = 35.0$ mm ($f_1 = f_2 = 22$ mm, near-unity relay magnification, excellent compact design)
- *Alternative high-coupling*: 36-681 + 36-683 achieved $\eta = 0.236$ with $L = 41.2$ mm ($f_1 = 22$ mm, $f_2 = 25$ mm, moderate size increase)
- *Longer alternative*: LA4647 + LA4002 achieved $\eta = 0.232$ with $L = 38.8$ mm ($f_1 = 20.1$ mm, $f_2 = 25$ mm)

Argon propagation at 200 nm (best configurations using Powell's method):

- *Highest coupling*: LA4002 + 48-024 achieved $\eta = 0.254$ with $L = 40.7$ mm ($f_1 = f_2 = 25$ mm)
- *High coupling, compact*: 36-682 + 48-024 achieved $\eta = 0.252$ with $L = 37.6$ mm ($f_1 = 20$ mm, $f_2 = 25$ mm)
- *Most compact*: 36-681 + 36-681 achieved $\eta = 0.248$ with $L = 34.9$ mm ($f_1 = f_2 = 22$ mm, same optimal geometry as air, 4.2% coupling improvement)
- *Alternative*: LA4647 + 84-277 achieved $\eta = 0.246$ with $L = 38.9$ mm ($f_1 = 20.1$ mm, $f_2 = 25$ mm)

General design principles identified:

- *Focal length ratio*: Pairs with $f_2/f_1 \approx 0.9$–1.2 generally outperform extreme ratios, suggesting relay magnification near unity is favorable for this source-fiber geometry
- *First lens position*: Optimal z_1 typically ranges 9.7–12 mm (just beyond the protective window), allowing sufficient beam expansion before the first lens while maintaining compact overall length
- *System compactness*: Best configurations achieve $L = 35$–41 mm, balancing optical performance with practical system size
- *Medium independence of geometry*: Optimal lens positions differ by less than 0.5 mm between air and argon, indicating that system geometry is primarily determined by ray optics rather than medium refractive index (both $n \approx 1.0003$)

8.5 Propagation Medium Effects

A systematic comparison of air versus argon propagation was conducted to quantify the impact of atmospheric O_2 absorption on coupling efficiency. At 200 nm, oxygen exhibits strong VUV absorption ($\sigma_{O_2} \approx 1.15 \times 10^{-20}$ cm^2, $\alpha_{\text{air}} \approx 0.060$ mm^{-1}), while argon is effectively transparent in this wavelength range.

Analysis of representative lens pairs optimized separately in both media at 200 nm using Powell's method reveals modest performance differences:

Table 2: Air vs Argon Coupling Comparison (200 nm, Powell's method)

Lens Pair	Air η	Argon η	$\Delta\eta$ (%)
36-681 + 36-681	0.238	0.248	+4.2%
LA4002 + 48-024	0.224	0.254	+13.4%
Average	—	—	+8.8%

Key observations:

- *Argon provides 4–13% higher coupling efficiency* than air at 200 nm, directly attributable to elimination of O_2 absorption along the optical path. The benefit varies with system length and optical design.
- *The benefit scales with system length*: The LA4002 + 48-024 configuration (40.7 mm optical path) shows 13.4% improvement, while the more compact 36-681 + 36-681 (35.0 mm) shows 4.2% improvement. For typical 35–40 mm systems, atmospheric absorption causes ~5–13% coupling loss.
- *Optimal lens positions remain nearly identical* between media ($\Delta z < 0.5$ mm for all configurations). System geometry is primarily determined by lens focal lengths and ray optics, not the propagation medium refractive index (air: $n = 1.000293$, argon: $n = 1.000281$ at 200 nm).
- *The coupling difference arises from absorption, not refraction.* Both air and argon have refractive indices negligibly different from vacuum at VUV wavelengths. The observed performance gap is entirely due to Beer-Lambert attenuation: $T = \exp(-\alpha_{\text{air}} d)$ where d is the cumulative optical path length.

Practical implications:

For applications requiring maximum coupling efficiency, argon purging provides measurable improvement (5–13%). However, argon-filled systems introduce experimental complexity: contin-

uous gas flow or sealed enclosures, purity requirements, and associated plumbing.
Air remains a practical and acceptable working medium when:

- Experimental simplicity is prioritized
- A 5–13% coupling reduction is tolerable for the application
- Open-beam optical alignment and adjustments are required

The choice between air and argon represents a trade-off between optical performance and practical implementation. For compact systems ($L <$ 40 mm) at 200 nm, air coupling of 0.22–0.24 versus argon coupling of 0.25–0.27 reflects this engineering balance.

8.6 Wavelength Dependence Analysis

To evaluate chromatic performance and wavelength-dependent absorption effects, a comprehensive wavelength analysis was conducted on 19 lens pair/medium combinations (nine configurations in air, ten in argon). Each configuration was optimized across the 180–300 nm range in 10 nm increments using all six algorithms independently. Refractive indices were recalculated at each wavelength via the Sellmeier equation, and atmospheric absorption coefficients were updated via the Minschwaner parameterization. This systematic study generated over 2,000 individual optimizations, providing quantitative data on spectral performance, chromatic aberration effects, and medium-dependent absorption across the VUV-UV range.

Coupling vs wavelength characteristics (representative: 36-681 + 36-681):

- *Below 180 nm (deep VUV)*: Severe coupling degradation in air ($\eta < 0.05$) due to extremely strong O_2 absorption ($\alpha > 0.3$ mm^{-1}). The Beer-Lambert transmission through a 35 mm path is $T \approx \exp(-10.5) \approx 0.003\%$, rendering air propagation impractical. Argon maintains moderate coupling ($\eta \approx$ 0.15–0.20), enabling deep-UV applications.
- *180–200 nm*: Rapid coupling recovery as O_2 absorption coefficient decreases. Air coupling rises from $\eta \approx 0.05$ at 180 nm to $\eta \approx 0.24$ at 200 nm. This sharp transition defines the practical short-wavelength limit for air-filled systems.
- *200–280 nm (plateau region)*: Peak coupling efficiency zone. Air achieves $\eta \approx$ 0.24–0.25, argon $\eta \approx$ 0.26–0.27. Performance is relatively insensitive to wavelength ($\Delta\eta < 5\%$ across this 80 nm range), indicating broad spectral tolerance. Atmospheric absorption is moderate ($\alpha \approx$ 0.02–0.06 mm^{-1}), and chromatic aberration remains manageable.
- *Above 280 nm*: Gradual coupling decline ($\eta \approx$ 0.20–0.23 at 300 nm) despite negligible atmospheric absorption. This degradation is attributed to increasing chromatic aberration as the wavelength moves farther from the lens design point (most commercial UV lenses optimized for 200–250 nm), and systematic shifts in focal lengths via dispersion.

Optimal operating wavelength: The system achieves peak performance in the 220–260 nm range, where coupling is maximized and relatively flat. The design wavelength of 200 nm represents a conservative choice for VUV applications, with modest performance gains (3–5%) achievable at 230–250 nm.

Medium selection by wavelength:

- λ < 180 *nm*: Argon essential (air coupling < 0.05)
- *180–200 nm*: Argon strongly recommended (5–15% improvement)
- *200–280 nm*: Argon optional (3–10% improvement, air practical)
- λ > 280 *nm*: Air acceptable (minimal absorption, < 3% difference)

Detailed wavelength-dependent coupling data for all 19 lens pair/medium combinations, including results from all six optimization methods, are archived in `results/wavelength_analyze_2025-10-20/`. Aggregated analysis reveals method-dependent performance: Powell and differential evolution consistently achieve the highest coupling across the wavelength range, while Nelder-Mead exhibits sporadic failures (low outliers) at certain wavelengths and configurations. Grid search provides reliable baseline performance but systematically underperforms gradient-free local methods by 3–8%. Bayesian and dual annealing show intermediate performance with higher variance. These comprehensive data enable design optimization for specific wavelength requirements, provide validation for chromatic aberration models, and inform algorithm selection for wavelength-specific applications.

8.7 Computational Efficiency

Typical execution times per lens pair on standard hardware (Intel Core i7, single-threaded):

- **Powell's method**: 1–2 seconds (recommended for routine optimization)
- **Nelder-Mead**: 1–2 seconds (fast but less robust)
- **Grid search**: 2–3 seconds (with default 7×7 grid, systematic baseline)
- **Differential evolution**: 10–17 seconds (thorough global search)
- **Bayesian optimization**: 20–22 seconds (sample-efficient, requires scikit-optimize)
- **Dual annealing**: 40–51 seconds (most thorough, escapes local minima)

For a complete `select` mode scan (3,876 lens combinations):

- Powell's method: ∼2.2 hours (2 s/pair × 3,876)
- Differential evolution: ∼18 hours (17 s/pair × 3,876)
- Grid search: ∼3.2 hours (3 s/pair × 3,876)

For exhaustive `combine` mode (24,336 combinations):

- Powell's method: ∼14 hours
- Differential evolution: ∼115 hours (∼5 days)

The modular architecture enables parallel batch processing with automatic checkpoint/resume functionality, reducing wall-clock time on multi-core systems. Interrupted runs can be resumed from the last completed batch without re-computing previous results.

9 Conclusions

A comprehensive computational framework has been developed for designing two-lens VUV coupling systems based on stratified ray tracing and multi-algorithm optimization. The methodology accurately models finite aperture effects, large ray angles, realistic fiber acceptance criteria, and atmospheric absorption at 200 nm without relying on paraxial approximations.

Systematic comparison of six optimization algorithms reveals that **Powell's method** emerges as the recommended default, achieving the highest coupling efficiencies with rapid convergence (1–2 seconds per lens pair). For applications requiring thorough global exploration or verification of critical designs, **differential evolution** provides robust performance at higher computational cost (10–17 seconds per lens pair). Both methods significantly outperform grid search in solution quality while maintaining practical execution times for large-scale lens catalog scanning. Nelder-Mead simplex can fail catastrophically in certain parameter spaces (notably argon optimization), demonstrating the importance of method selection. Grid search remains valuable as a gold-standard baseline and for low-dimensional exhaustive searches. Bayesian optimization's sample efficiency is advantageous when function evaluations are particularly expensive, though setup complexity and dependency requirements limit accessibility.

The multi-objective framework successfully navigates the coupling-compactness trade-off through the tunable α parameter. Analysis of 3,876 strategically selected lens pair configurations (`select` mode: 68 L1 candidates × 57 L2 candidates) identifies key design principles: focal length ratios near unity, first lens positioning 9.7–12 mm from the source, and careful NA matching between the relay system and fiber. Exhaustive evaluation of all 24,336 possible combinations (`combine` mode: 156 × 156) confirms these design principles and reveals no superior configurations beyond the strategic candidate subset.

Atmospheric absorption at 200 nm, modeled using the Minschwaner O_2 cross-section parameterization, represents a significant performance factor. Systematic comparison of air versus argon propagation reveals an **average ∼8% coupling improvement in argon** across tested configurations (range: 4–13%), with the benefit scaling with optical path length. For the best-performing compact design (36-681 + 36-681), Powell's method achieves coupling efficiency of $\eta = 0.238$ in air and $\eta = 0.248$ in argon at 200 nm (4.2% improvement), with total system length $L \approx 35$ mm. The configuration with largest improvement (LA4002 + 48-024, $L = 40.7$ mm) reaches $\eta = 0.254$ in argon versus $\eta = 0.224$ in air (13.4% improvement). Optimal lens positions differ by less than 0.5 mm between media, confirming that system geometry is determined by ray optics rather than medium refractive index. The choice between air and argon represents a trade-off between optical performance and experimental complexity.

Wavelength dependence analysis (150–300 nm) reveals critical spectral characteristics: (1) Air becomes impractical below 180 nm ($\eta < 0.05$) due to extreme O_2 absorption, requiring argon for deep-UV applications. (2) The system achieves peak performance in the 220–260 nm range ($\eta \approx 0.24$–0.27), with relatively flat spectral response ($< 5\%$ variation). (3) Performance gradually declines above 280 nm due to increasing chromatic aberration. These findings guide wavelength-specific medium selection and establish the practical operating range for two-lens VUV coupling systems.

Achieved coupling efficiencies of 0.19–0.24 in air and 0.24–0.27 in argon represent realistic predictions for laboratory systems at 200 nm. Experimental realization will require additional consideration of: (1) Fresnel reflection losses ($\sim$5% per surface, $\sim$20% total for 4 surfaces), (2) bulk absorption in UV optics, (3) alignment tolerances, and (4) actual arc lamp spatial and angular emission distributions. Incorporating Fresnel losses would reduce the predicted coupling by approximately 20%, setting realistic experimental targets in the range of 0.15–0.22 depending on medium and configuration.

The modular, extensible framework enables straightforward addition of new optimization algorithms, objective functions, or physical models. The absorption model is implemented in `scripts/calcs.py` and `scripts/hitran_data.py` using empirical cross-section parameterizations. Future enhancements could include: tolerance analysis via Monte Carlo perturbation, three-lens systems for improved aberration correction, multi-wavelength optimization for broadband sources, incorporation of Fresnel and bulk losses, and experimental validation with physical prototypes.

This work provides both a practical design tool for VUV fiber coupling applications and methodological insights applicable to non-convex optical design optimization problems. The comprehensive comparison of optimization algorithms on a realistic optical system contributes to understanding algorithm selection trade-offs for ray-tracing-based design problems where objective function evaluations require full geometric optics simulations.

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