Parallel Hybrid Optimization Algorithm for the Material Composition of Multilayer Thin-Film Structures

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Objective

To create a method for the design of multilayer thin-film structures that:

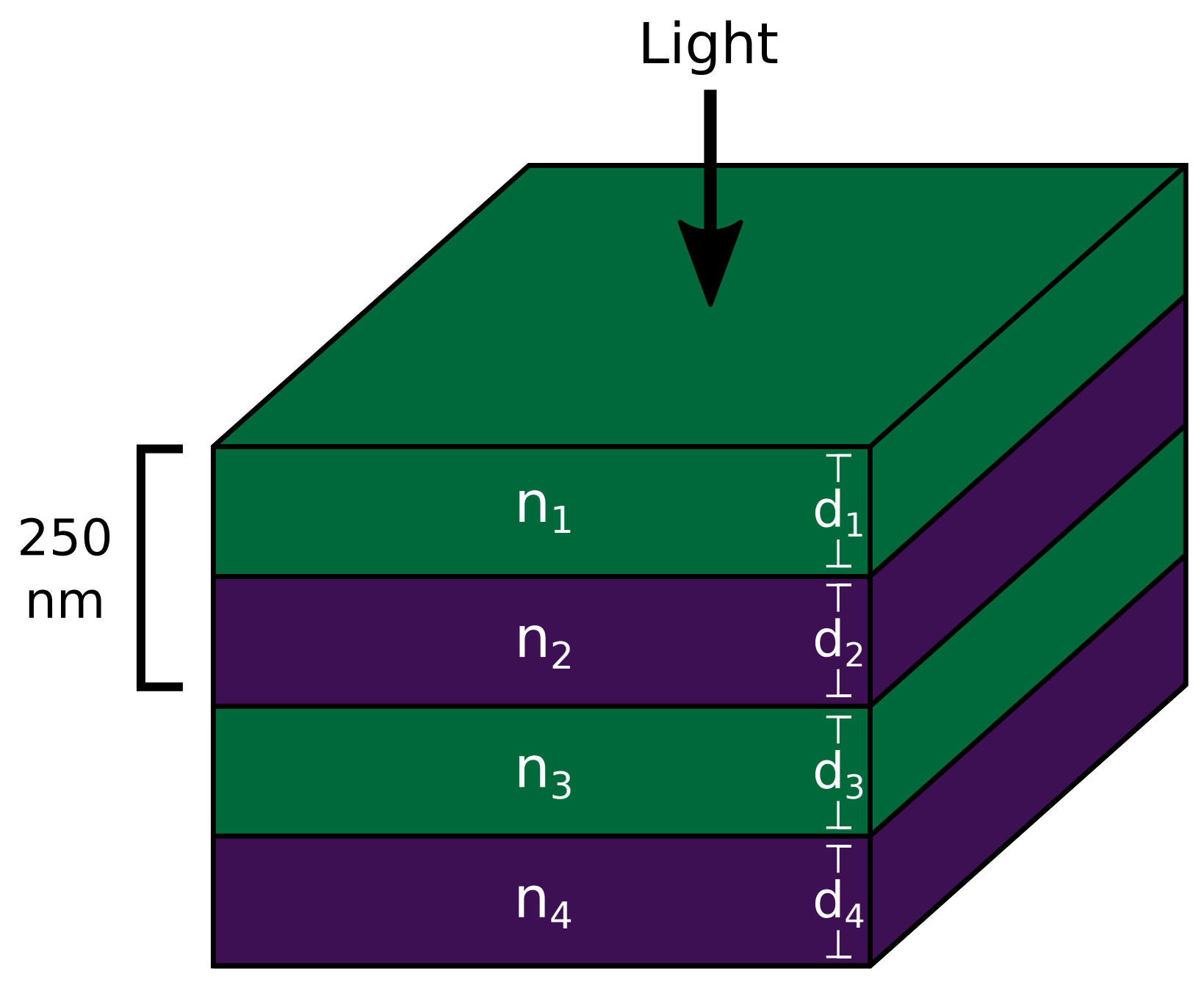
- Improves upon existing general-purpose optimization algorithms.
- Supports parallelization.
- Chooses both layer thickness and material.

Introduction

Multilayer thin-film structures consist of sub-micron layers of materials with differing optical properties. These structures exhibit optical interference effects, having applications as optical coatings: anti-reflective coatings, mirrors, filters, and more [1].

Calculating the optical spectra of these structures is well-defined mathematically, but they have too many parameters to solve analytically in many cases. Structures are designed for specific applications using computational numerical methods.

Prior work has applied general-purpose mathematical optimization techniques to structure design, but design commonly uses domain-specific techniques and focuses on the optimization of thicknesses, not materials. **This work seeks to improve upon past attempts using general-purpose algorithms and parallelization.**

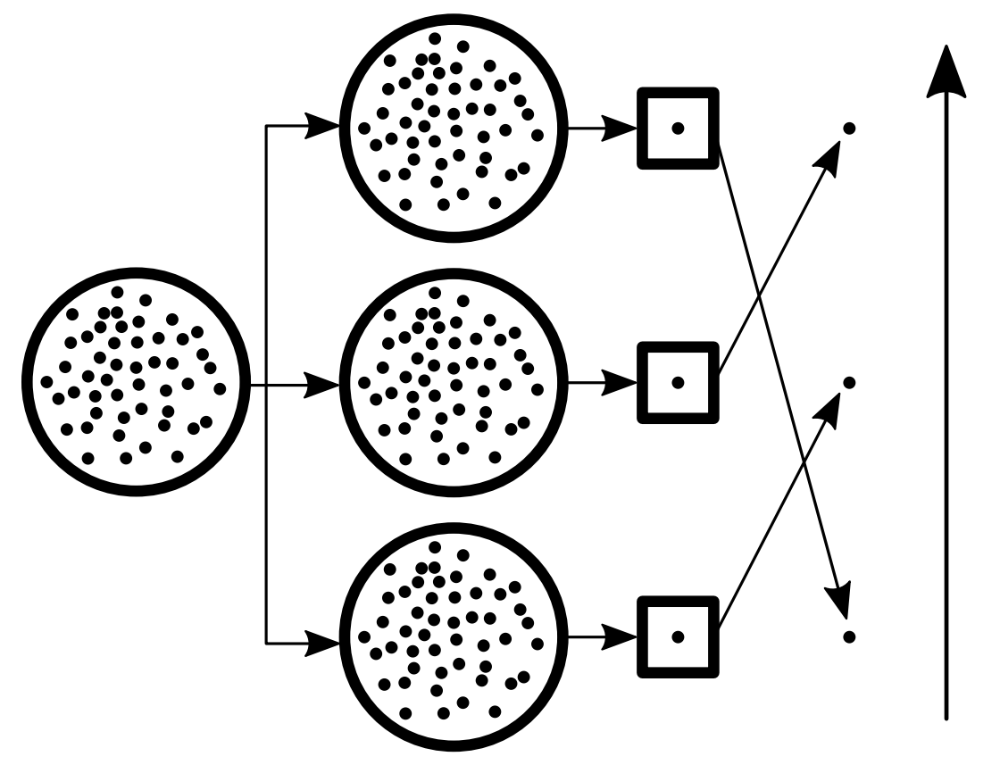


An abstract multilayer thin-film structure. Layer thicknesses and material refractive indices completely characterize a structure.

Algorithm

A hybrid optimization algorithm was designed both to yield better results than comparable evolutionary methods and to support parallelization. It consists of three stages:

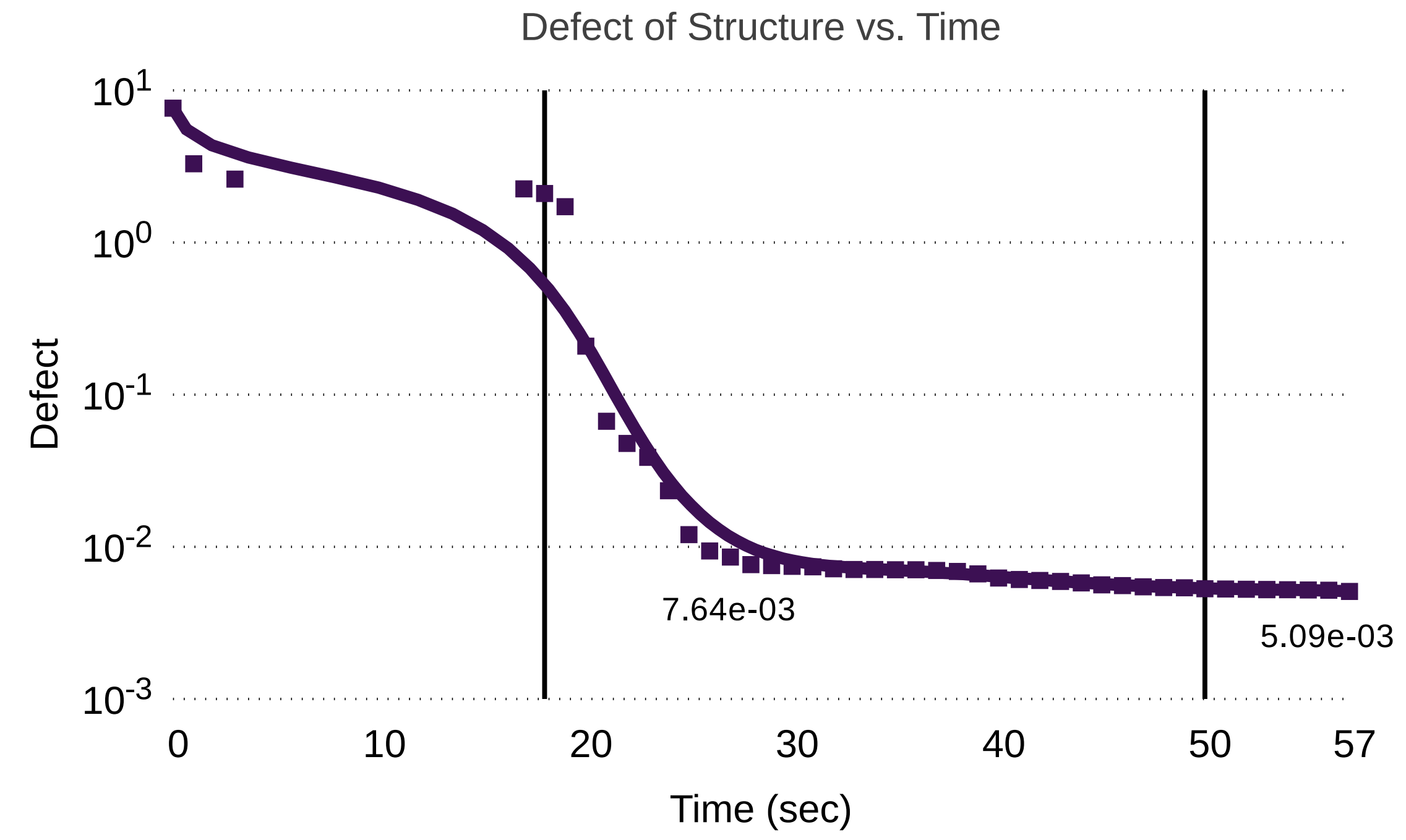
- **Monte Carlo simulation**: random search to identify viable material compositions
- **Continuous, adaptive genetic algorithm**: optimize thicknesses for each material set
- **Pattern search**: locally minimize best results



Algorithm flow diagram. First, the best of many randomly generated structures are chosen. Each seeds a "population" with its materials, and thicknesses are optimized. The best of each population is improved, and results are sorted.

Improved Results

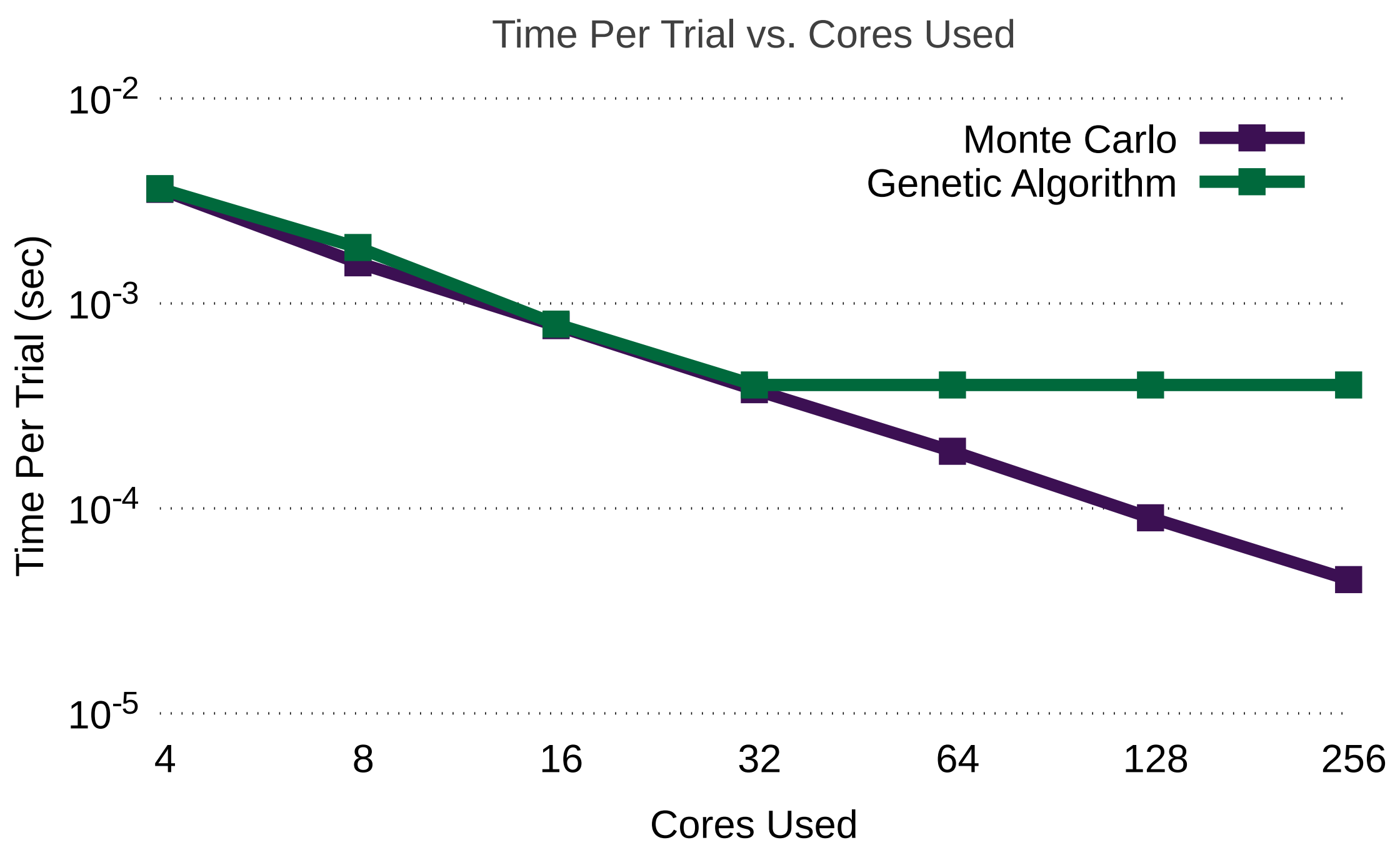
The algorithm was tested on a sample anti-reflective coating design problem [2]. Results were judged by evaluating their defect value, a linear measure of their difference from the ideal result. **The algorithm improved upon a prior result [2, pp. 593] by 3.3% while running for 57 seconds.**



Improvement of structure by algorithm. The three stages of the algorithm are separated by vertical lines. Run on 64 cores.

Parallel Performance

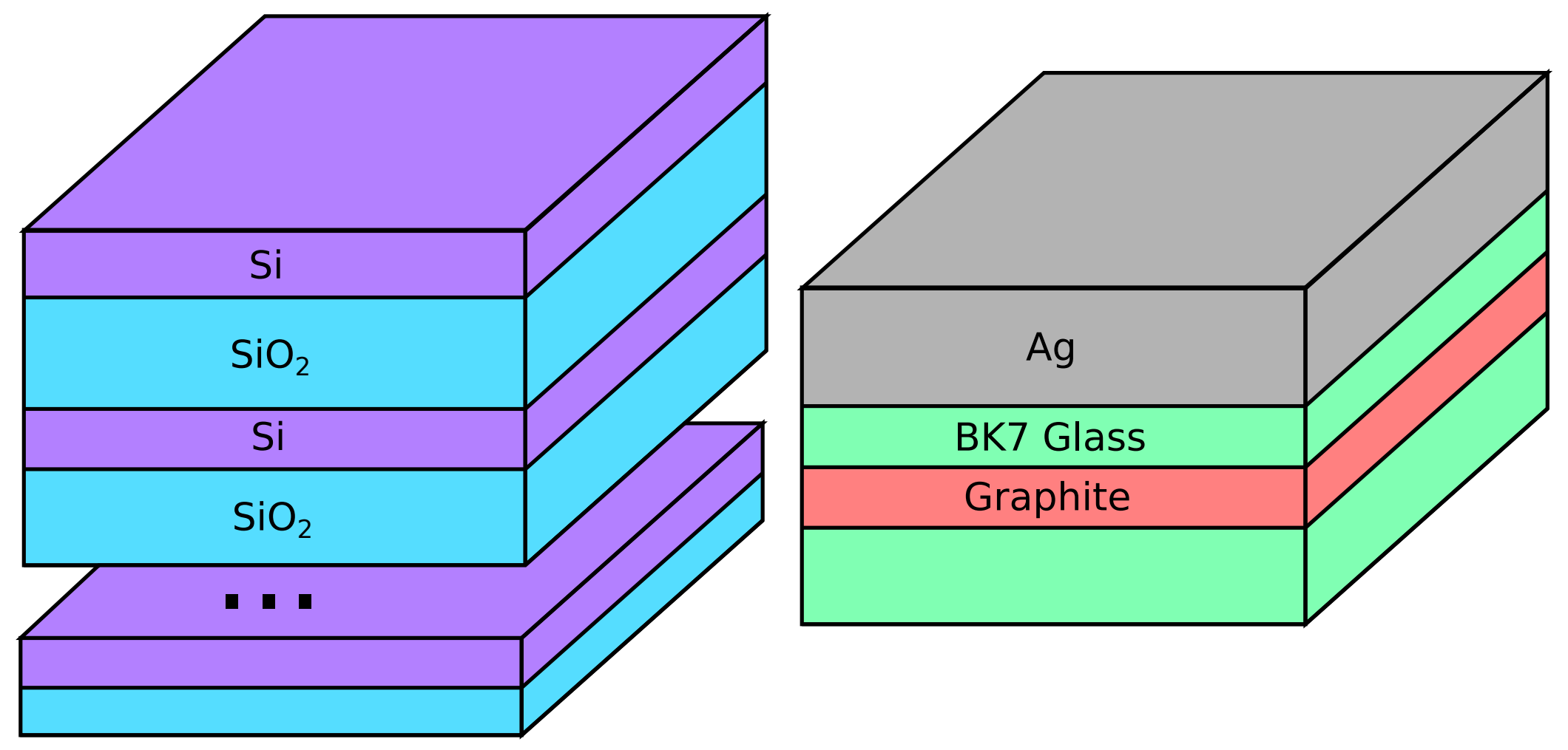
The sample design problem [2] was tested on increasing numbers of CPU cores. **The time per trial decreases linearly as cores used increases**, unlike existing unparallelized algorithms. The plateau in genetic algorithm performance improves when structures are larger or when more structures are tested.



Algorithm speedup from parallelization. Simulations run on the SuperMike-II cluster. Genetic algorithm normalized by trials per "generation" of the algorithm.

Material Optimization

A potential application of the algorithm is for the design of reflectionless structures that absorb or transmit all light at a given wavelength. An existing example of such a structure was designed using sixteen layers [3]. The algorithm instead created one using four layers by choosing materials itself. **This reduced normalized reflectance at the target wavelength (532nm) from 1.9×10^{-3} to 1.0×10^{-6}.**



Comparison of traditionally-designed structure to structure designed by new method.

Conclusion

The new method for multilayer thin-film structure design shows improvement over prior results in preliminary tests. Applications to existing problems show improved results, linearly improved performance through parallelization, and proof of concept that materials can be algorithmically chosen.

Future Work

- Test the method on more classes of problems to statistically study algorithm effectiveness.
- Reduce synchronization during genetic algorithm to improve parallel speedup.
- Explore other methods for choosing materials.

References

[1] J. D. Joannopoulos *et al.*, *Photonic Crystals* (Princeton University Press, 2008), 2nd ed.

[2] A. J. Thelen and R. Langfeld, "Coating design contest: antireflection coating for lenses to be used with normal and infrared photographic film," (1993), vol. 1782 of *Proc. SPIE*, pp. 552–601.

[3] L. Feng *et al.*, "Demonstration of a large-scale optical exceptional point structure," Opt. Express **22**, 1760–1767 (2014).

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