Accelerating meta-atom design with optimization, inverse design and AI methods: an application oriented benchmark

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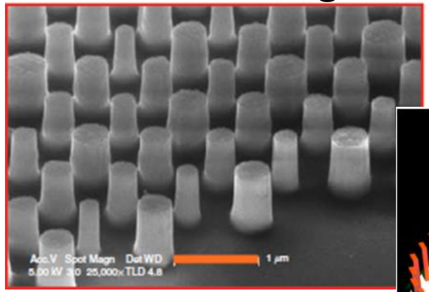
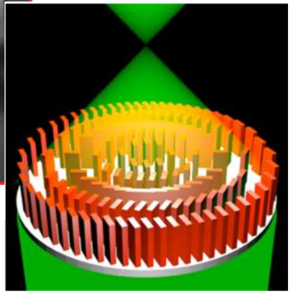
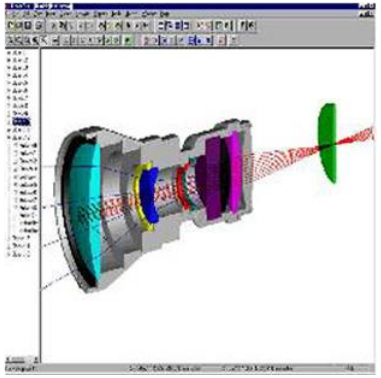
Nano-scale design



Component design



System Integration



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Bottlenecks in meta-surface design

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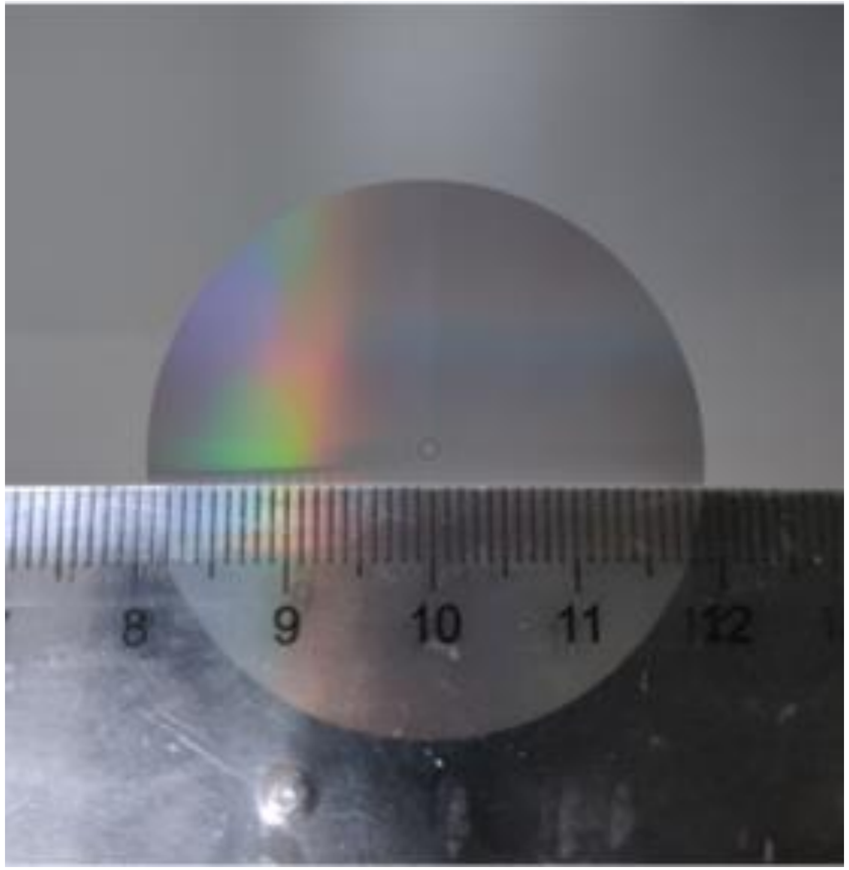
- Nano-structure full wave solution
  - All full wave algorithms scale poorly vs. DOF
  - Calculation times run into days to weeks easily
- Large area:
  - Memory limitations
  - Multi-scale methods increase the limit but require approximation
- Integration to system level
  - Link from wave to ray scale not well developed
  - Current models ignore higher order diffraction and amplitude



40mm diameter metalens

Example on-demand estimate for production (USD):*

- License server (t3.nano, 10 GB storage): $5/month
- Compute instances (**4 x c5n.18xlarge**, 20 GB storage each): **$11,360/month, $16/hour**
- Shared storage (EFS, **1 TB** usage): $300/month

*Estimate fromLumerical

Speeding up nano-structure search

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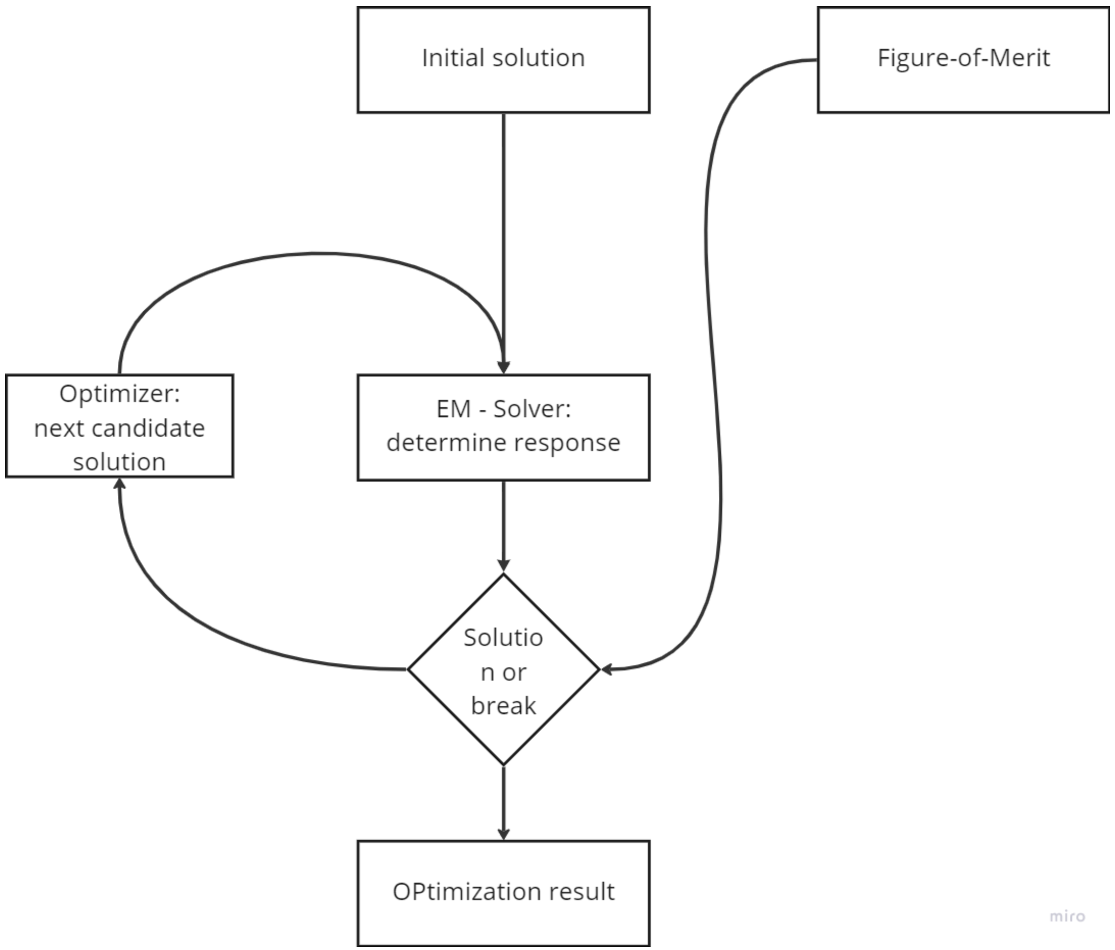
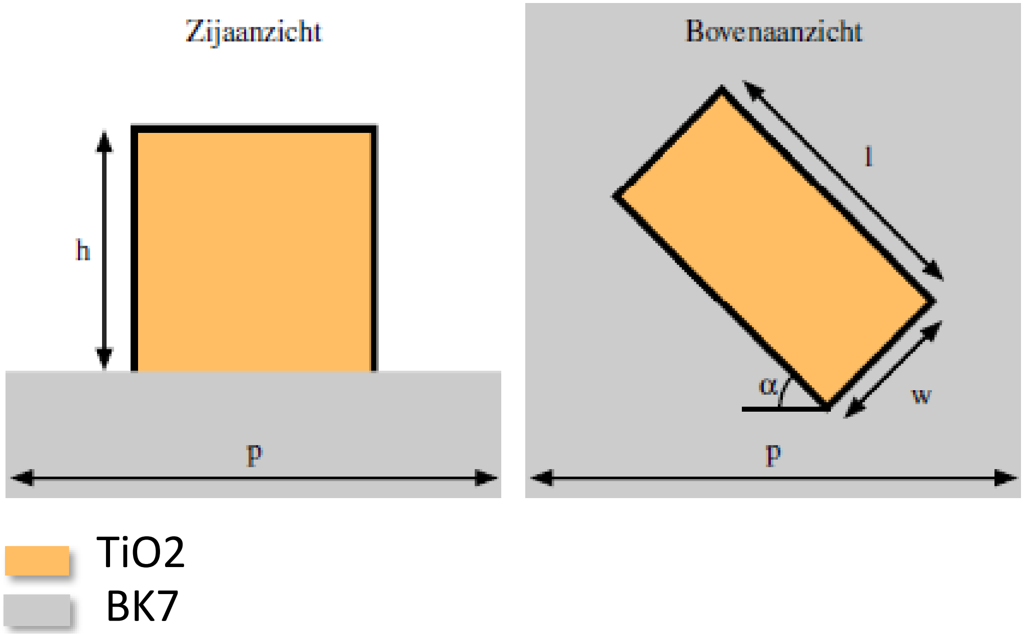


- Most time consuming aspect of design is the simulation of nano-structures
  - Typical: several **10 000s of structures**
  - Parametrized structures
  - Arbitrary shape structures
- Design contains a solver and an optimization loop
  - **Time spent = #calls x loop time**
  - Loop time determined by EM solver
- Two approaches to speed up:
  - Reduce #calls: smartest optimization alogrithm
  - Reduce loop time: fastes solver
- “Orthogonal” approaches can be combined

Ampbell, S. A. D. C., Ell, D. A. S., Enkins, R. O. P. J., Ric, E. B., Hiting, W., An, J. O. A. F., & Erner, D. O. H. W. (2019). Review of numerical optimization techniques for meta-device design. *Optical Materials Express*, *9*(4), 1842–1863.

Reference problem



- Reference problems:
  - Optimization of Pancharatnam Berry phase structures
- Standard design approach
  - Library of 32 structures
  - Fixed height and unit cell
  - TiO2 on glass
  - Wavelength 633nm
  - Period: 430nm
- Benchmark:
  - Brute force parameter sweep
  - Particle Swarm Optimization
  - Genetic Algorithm
  - Differential evolution
  - Covariance Matrix Adaptation Evolution Strategy
  - Bayesian optimization

Optimization: methods

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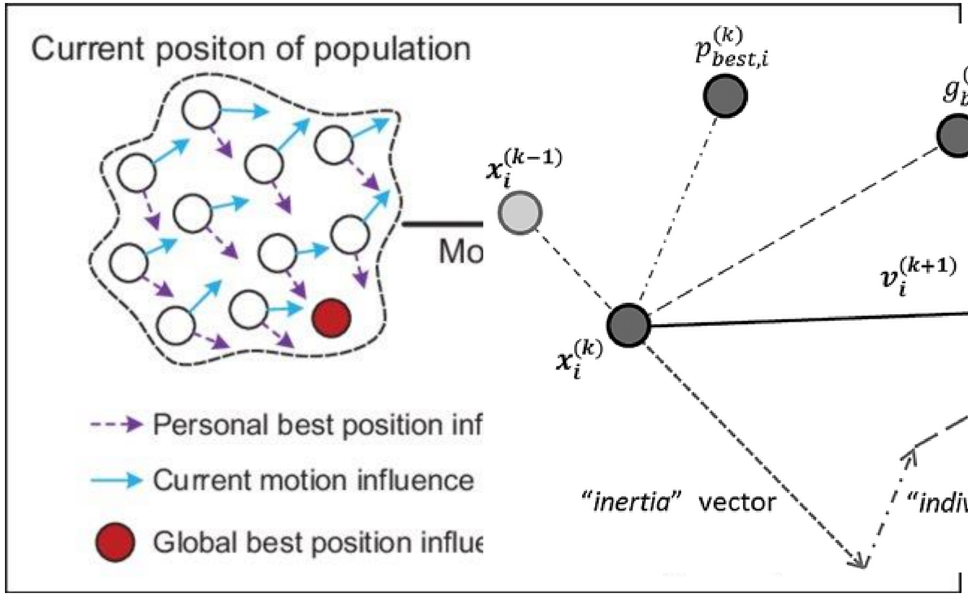
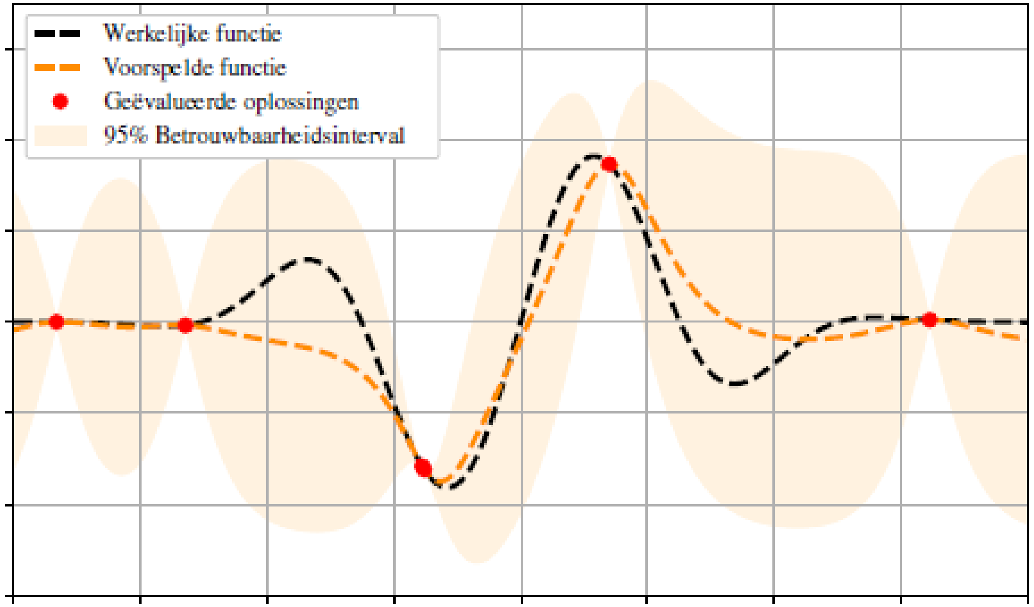


Particle swarm optimization (PSO)

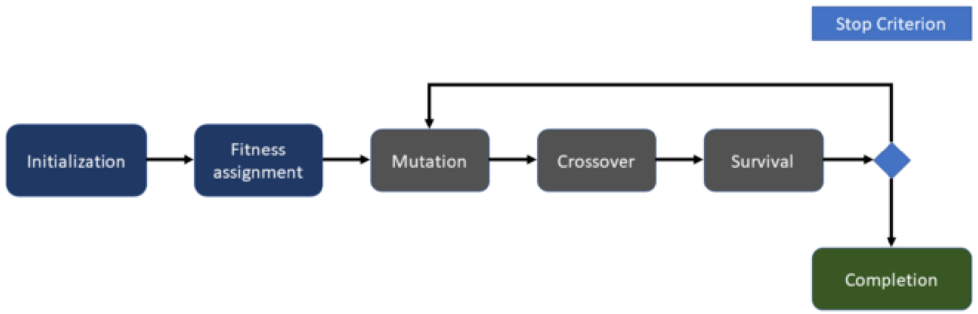
- Multiple starting points
- Direction of particle controlled by:
  - Best solution of all particles
  - Best position of individual particle
  - Momentum of individual particle



Bayesian Optimization

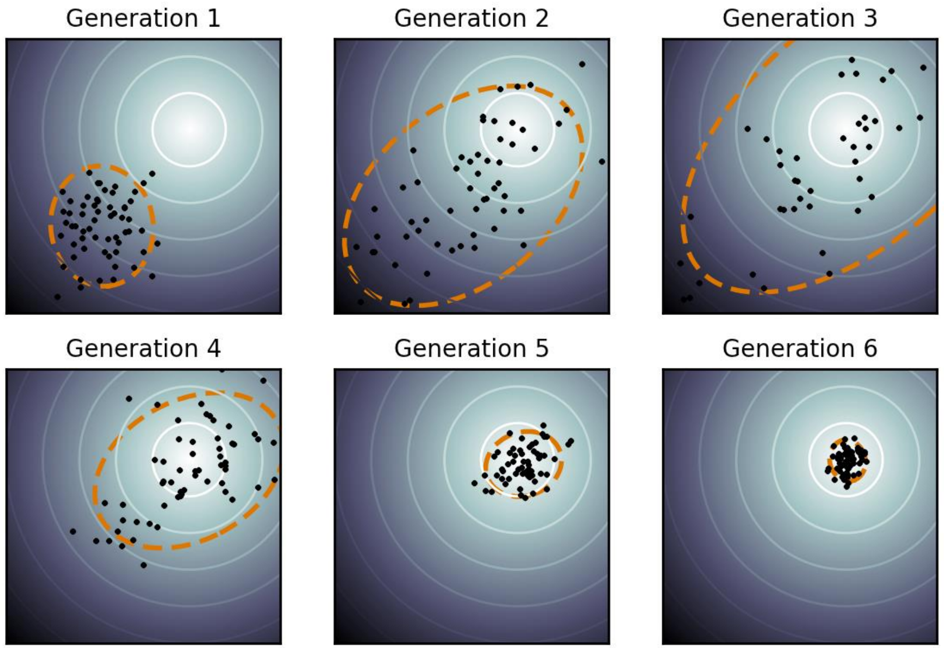
- Constructs a polynomial approximation of the error landscape from previous iterations
- Analytical solution of appriximate polynomial error landscape

Optimization: methods



Genetic algorithm (GA) and **Differential evolution** (DE)

- Multiple starting points (population)
- Evolution over multiple iterations
  - Best solutions kept
  - Best solutions are changed by :
    - Cross-over
    - Random mutation



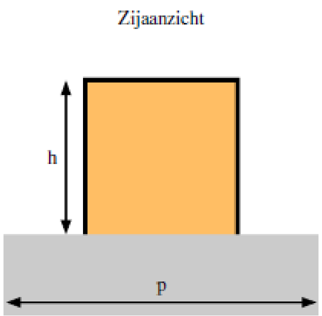
Covariance Matrix Adaptation Evolution Strategy (CMAES)

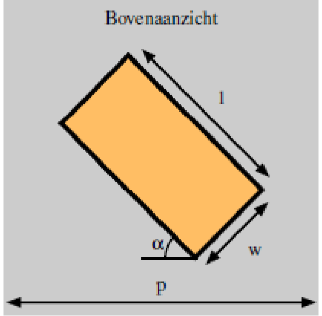
- Sampled solutiuons via normal distribution
- Evolution over multiple iterations
  - Best solutions kept
  - Search area expanded/decreased based on rate of change

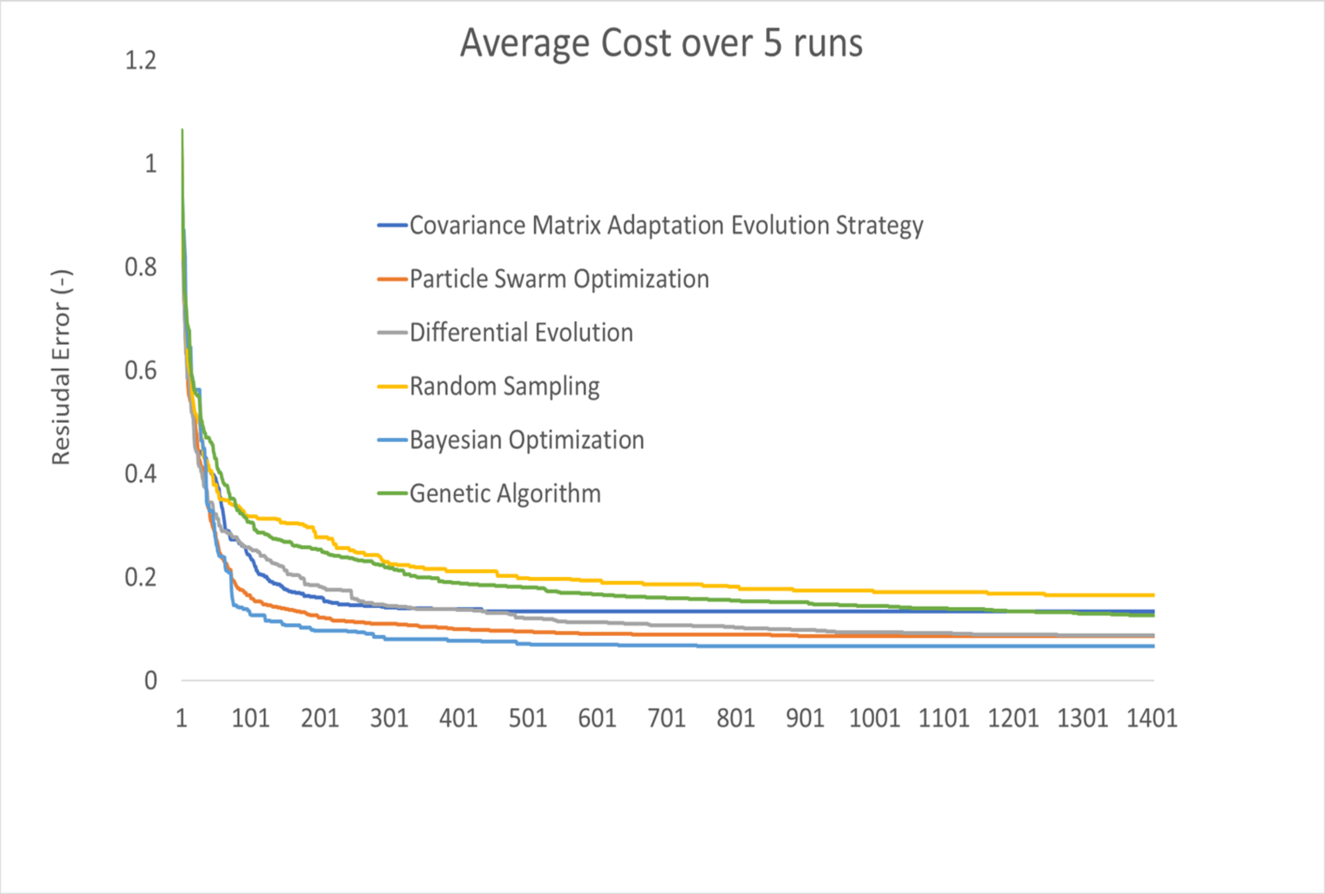
Benchmark results

- Pancharatnam Berry structure optimization
- Convergence reached in 400-1500 solver calls
- Error defined as $\varepsilon = |t - t_{target}|$

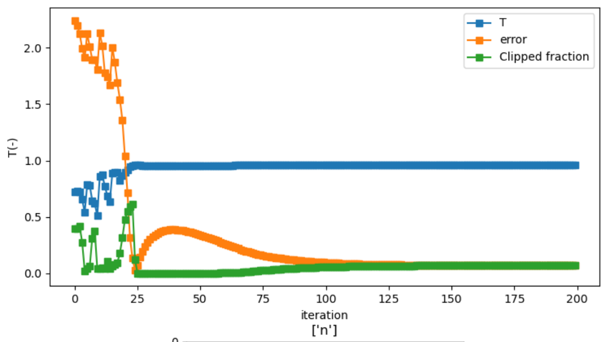
Algorithm	Final error	#calls to converge
Bayes	0,066	485
PSO	0,086	509
DE	0,0878	917
GA	0,126	1123
CMAES	0,133	245

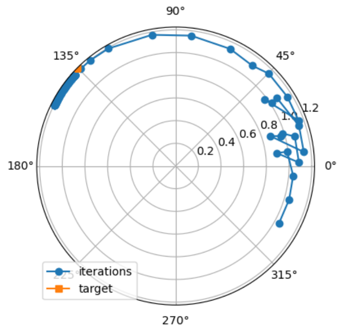


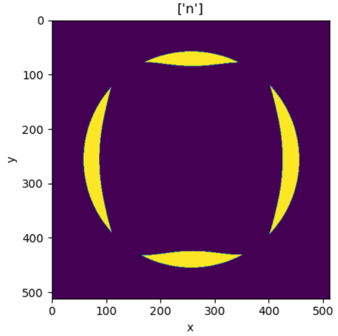


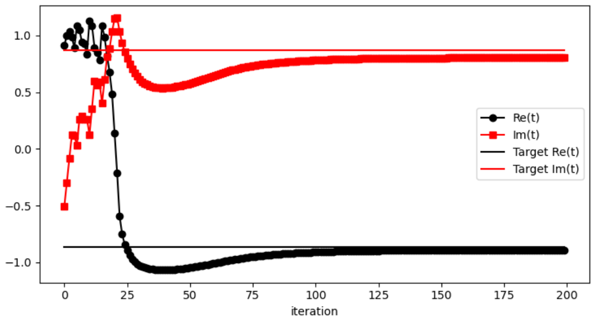


Adjoint optimization







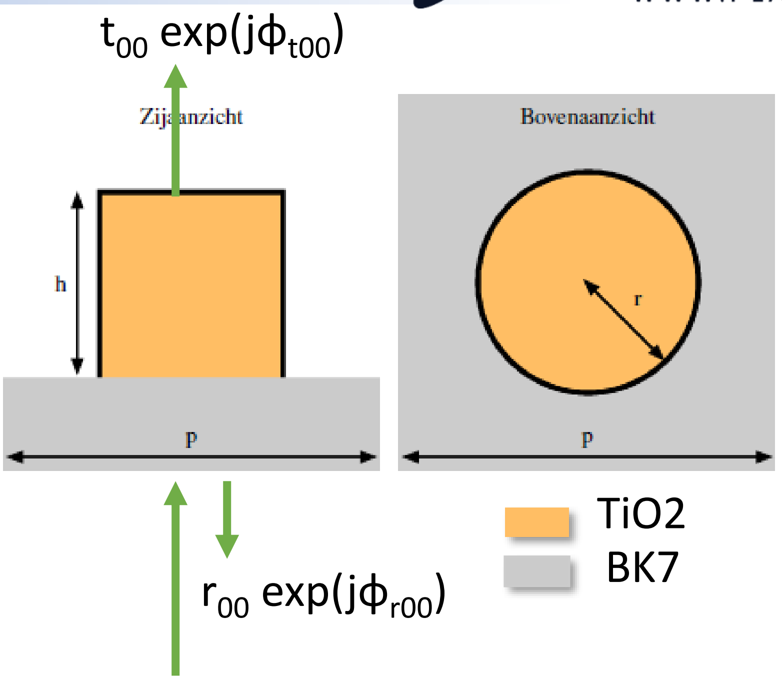


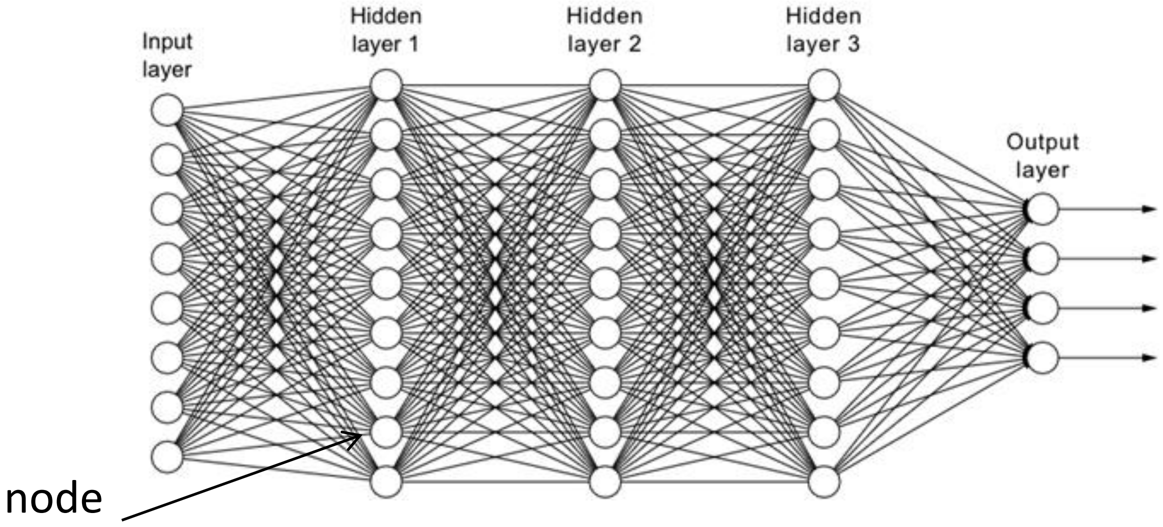
Algorithm	Final error	#calls to converge
Adjoint Optimization	0,05	200
Bayes	0,066	485
PSO	0,086	509
DE	0,0878	917
GA	0,126	1123
CMAES	0,133	245

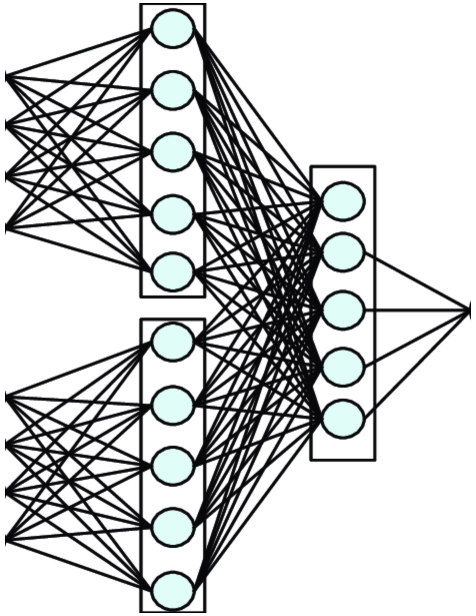
- Adjoint optimization
  - 2 solver calls per optimization
  - Gradient descent optimization
- Needs post-processing for:
  - Binary material distribution
  - Realistic feature sizes
- Post processing limits convergence and final result

Surrogate solver

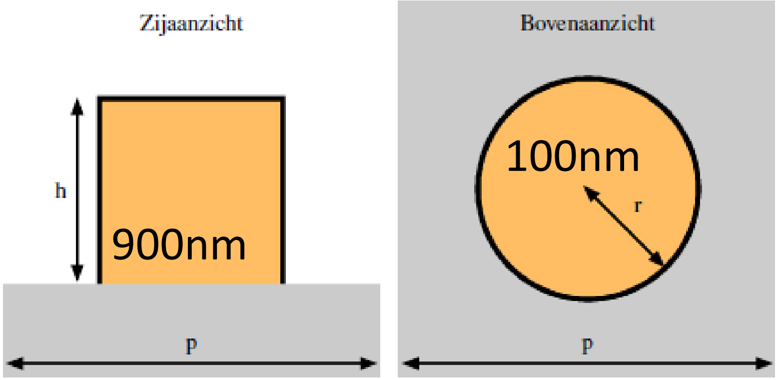
- Neural networks trained to predict RCWA solver answers
  - Reflected and transmitted phase and amplitude
  - Fundamental order (00)
- Physical parameters
  - Period P
  - Height H
  - Radius r
  - TE/TM
  - λ: 450-700nm







Surrogate NN results: example result



TiO2
BK7

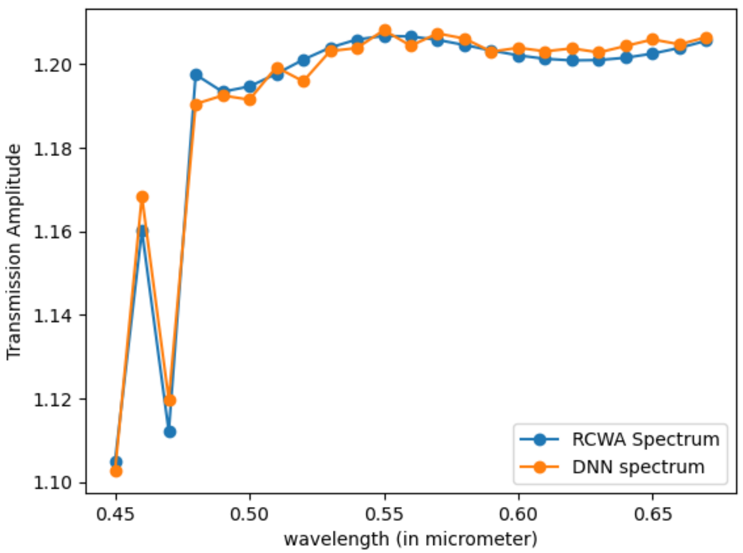
500nm

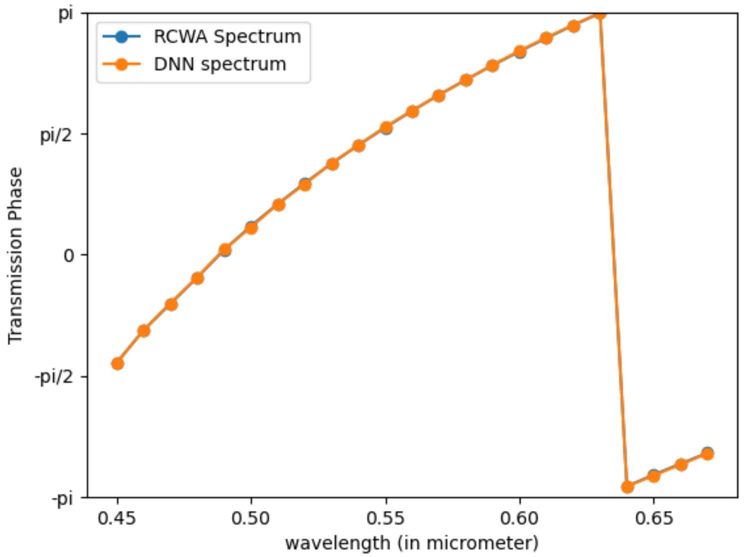
- DNN reproduces transmission and reflection
- Amplitude and phase reproduced
- Error metric: Euclidian distance

$$SE_{r/t} = |r/t_{NN} - r/t_{RCWA}|^2$$

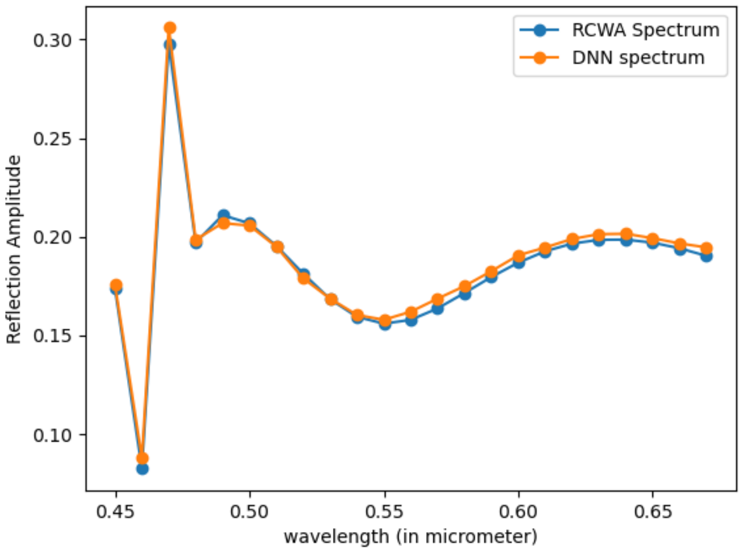
Direction	MSE	Mean Error
Transmission	7,2 10-5	0,85%
Reflection	5,6 10-5	0,75%

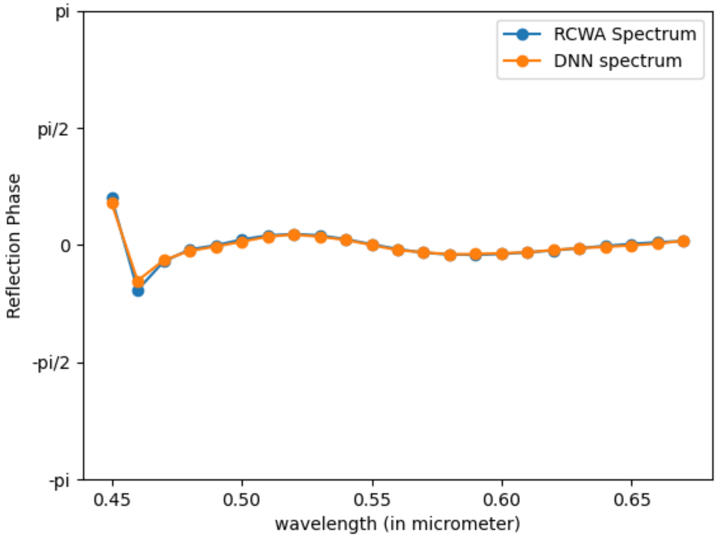
Transmission



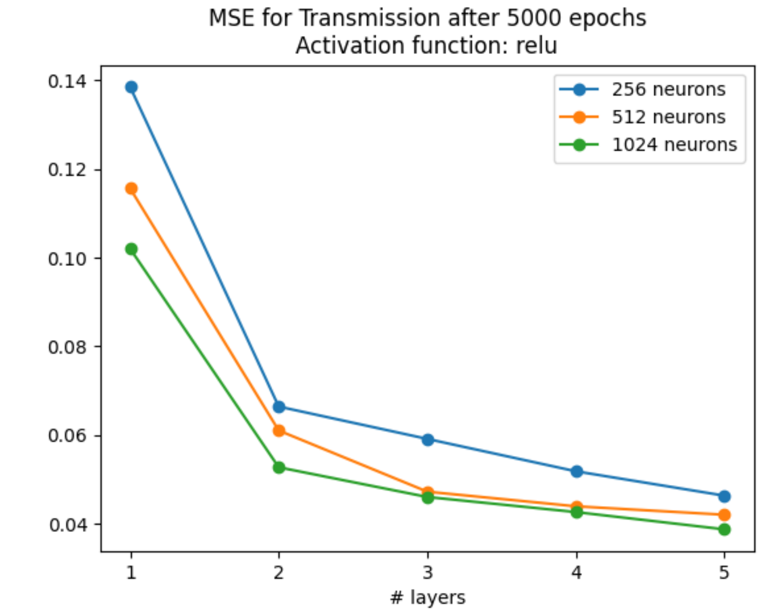


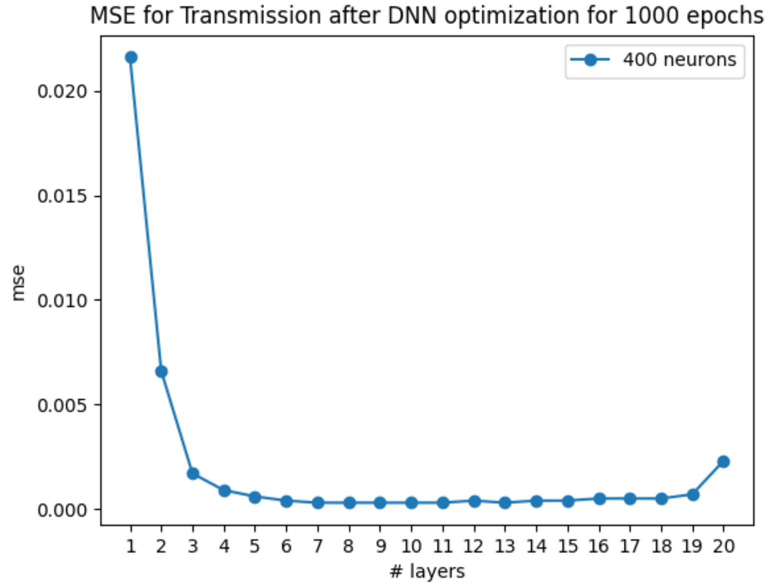
Reflection



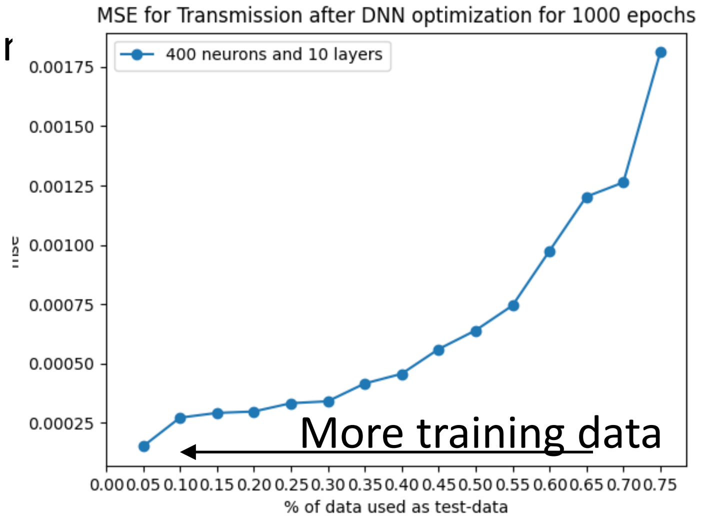


Effect of network choice

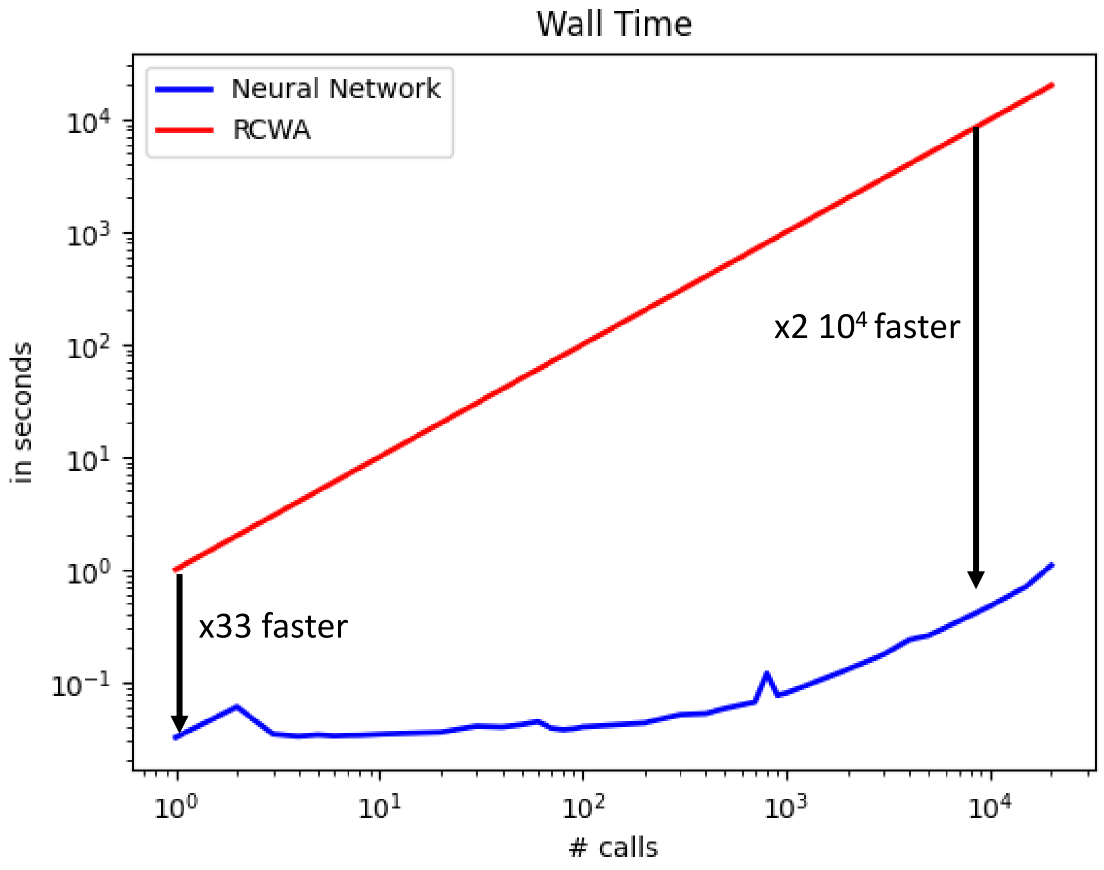




- ❖ Sufficient network complexity needed
  - ➢ Layers
  - ➢ Neurons per layer
- ❖ Neural Network types:
  - ➢ Fully connected layers
  - ➢ Shared layer network
  - ➢ Neural tensor layer
  - ➢ #nodes and # layers optimized
- ❖ Training data:
  - ➢ Large amount : 14
  - ➢ Representative sar



But is it faster?

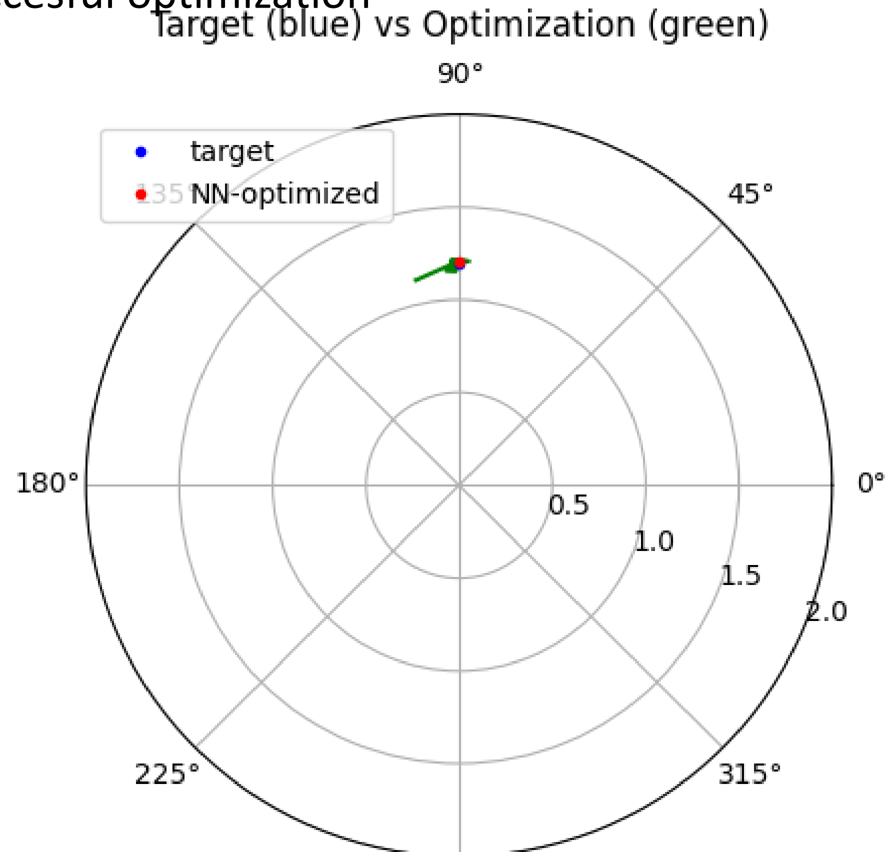


- Surrogate NN is 33 – 20 000 times faster than direct RCWA call
- 1 call (0,033s) 33x faster
- 9000 parallel calls (0,44s) -> 20 000 times faster

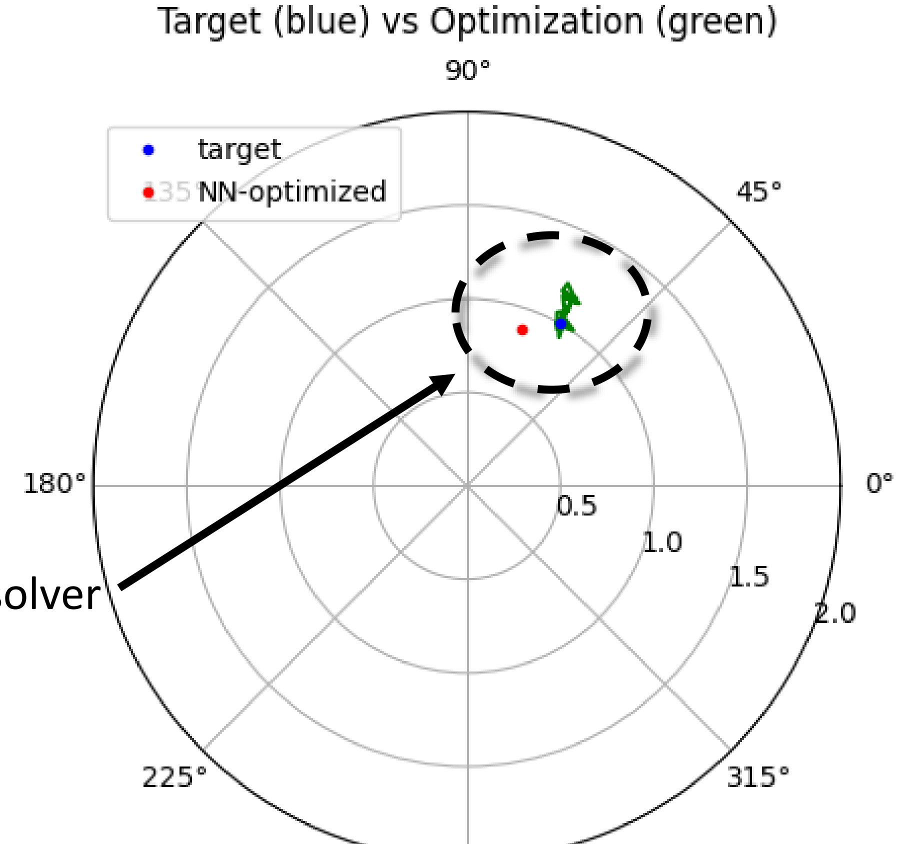
Surrogate solver + optimization

- Seacrh via genetic algorithm combined with surrogate solver
- Direct implementation: 31sec
- Optimized for large batches: 4,5sec

Succesful optimization



Unsuccesful optimization



Surrogate solver error

Conclusions

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- **Surrogate solver** and **optimization methods** can be used to **speed up** meta-atom design **up to 500 fold**
- **PSO, Bayesian** and **adjoint** method are **most performant optimization** algorithms
- Surrogate needs a pre-trained and accurate network. **Training takes more time** than a **classical design**.
- Surrogate only applicable to pre-defined material platform (substrate + material)

	#solver calls	Time per call	Total calculation time	Acceleration factor
Brute force sweep	64 000	1.1s	**19.55hr**	1 (baseline)
Parameter optimization (Bayesian)	32 000	1.1s	8.9hrs	2
Neural network training	400 000	1.1s	122hrs	0.16
Brute force pre-trained surrogate	64 000	0.03s	0.53hrs	37
Genetic + pre-trained surrogate	32 000	0.03s	0.27hrs	72
Brute force pre-trained surrogate	32 000	0,005s	**0,04hrs (3mins)**	**488**

Contact info

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