

Inverse Design Schemes for Light Propagation in Synthetic Media with Self-Induced Response

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Abstract

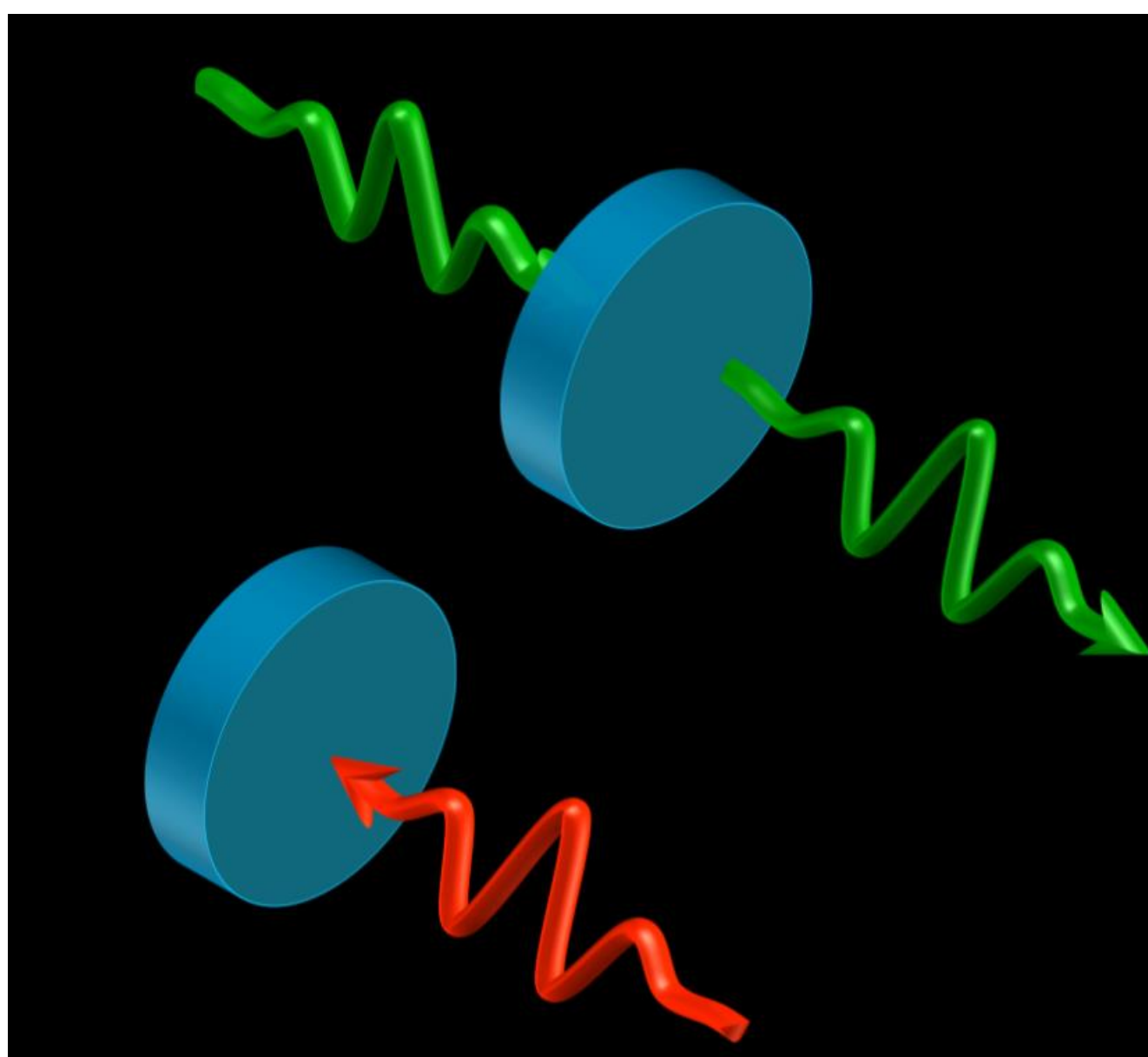
The traditional approach to realizing a device typically relies on familiar materials and geometries, guided by some derivative notions about the underlying physical mechanisms. Recently, the confluence of additive manufacturing, computer numerical control (CNC) machining and advanced computational paradigms such as *inverse design* is poised to reveal a plethora of enhanced architectures and novel structural platforms, useful in various areas of science and technology and covering every possible resolution domain from nano to macro-scale. In contrast to the traditional direct approach, inverse design starts from a target functionality and arrives at the optimal materials and geometries by quantitatively exploiting the full physical model under consideration with the aid of numerical tools such as heuristic search procedures like genetic algorithms or large-scale gradient-based adjoint optimization, as well as state-of-the-art machine-learning techniques such as artificial neural networks.

This project aims to develop an inverse design computational scheme that customizes electromagnetic transport in non-linear media. Our goal is to implement this method for the realization of a broad class of photonic devices like reflective limiters with broad-band low incident power transmittance, broad-band isolators, high-efficiency up/down frequency converters for night vision, or even invisibility cloaks.

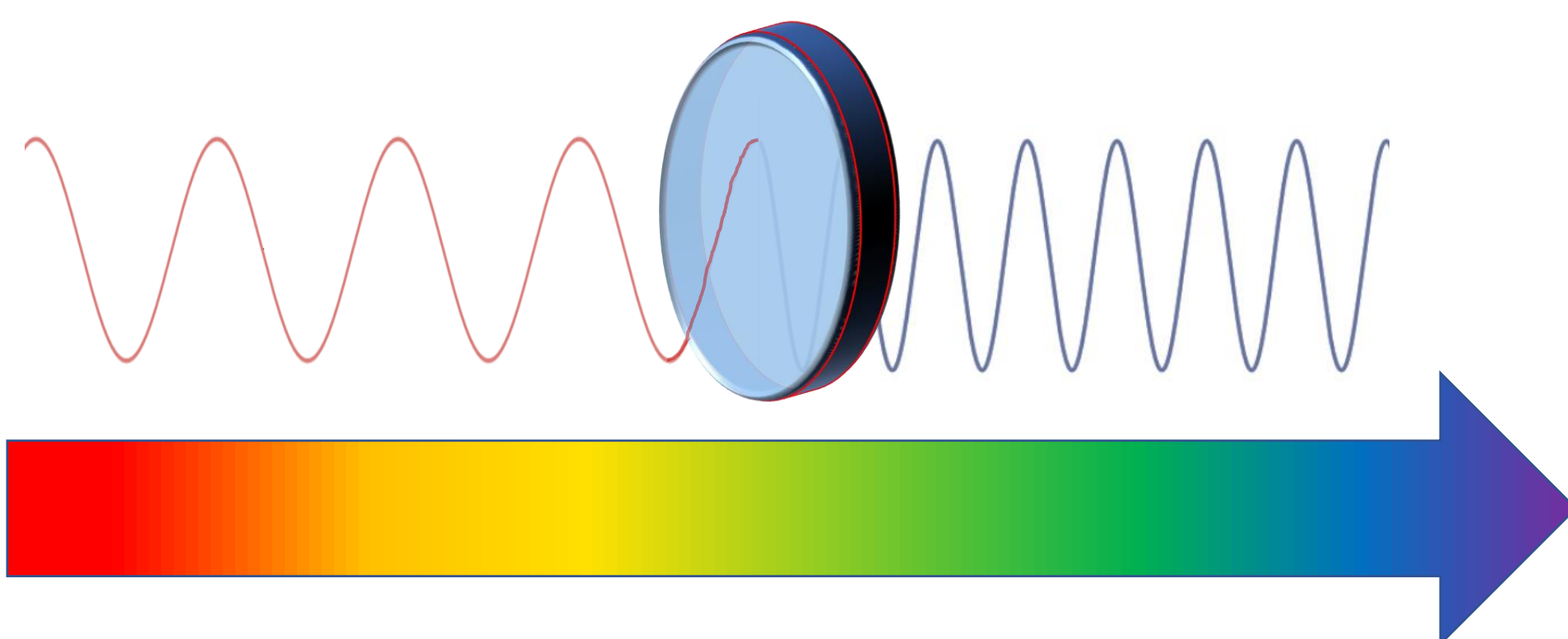
Motivation

The Adjoint Method of inverse design will allow us to cheaply invent geometries of novel photonic devices which serve as high-efficiency alternatives to existing designs.

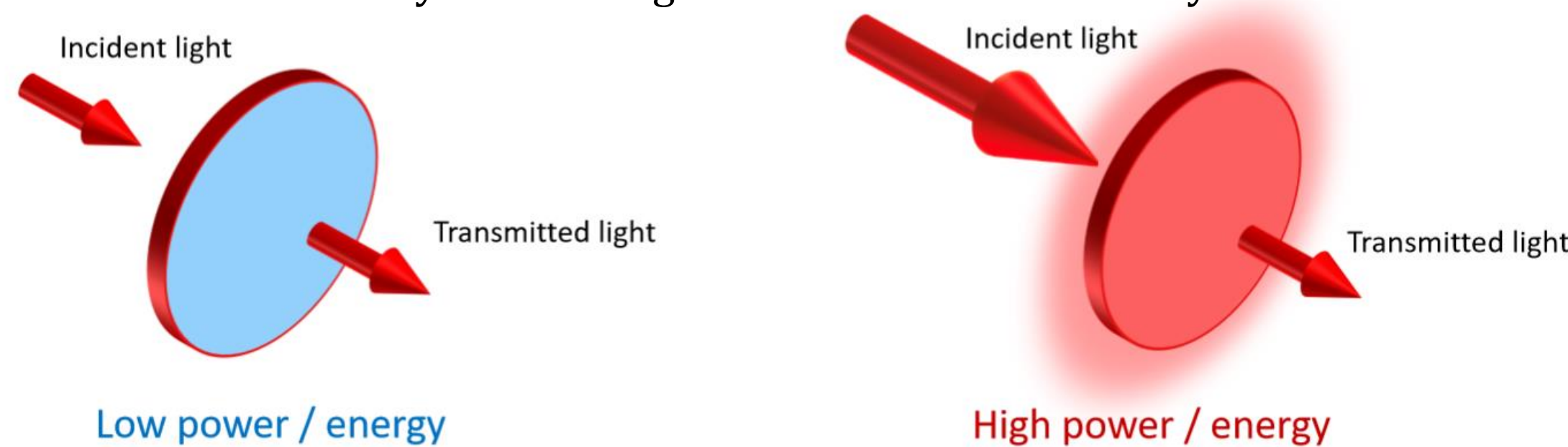
Optical isolators allow transmittance in only one direction



Upconverters accept incident light of low frequency and produce higher-frequency waves at the output



Limiters only transmit light below a certain intensity threshold:



Narrow-band limiters are common, though a broad-band limiter has not yet been invented.

[1]

Adjoint Method

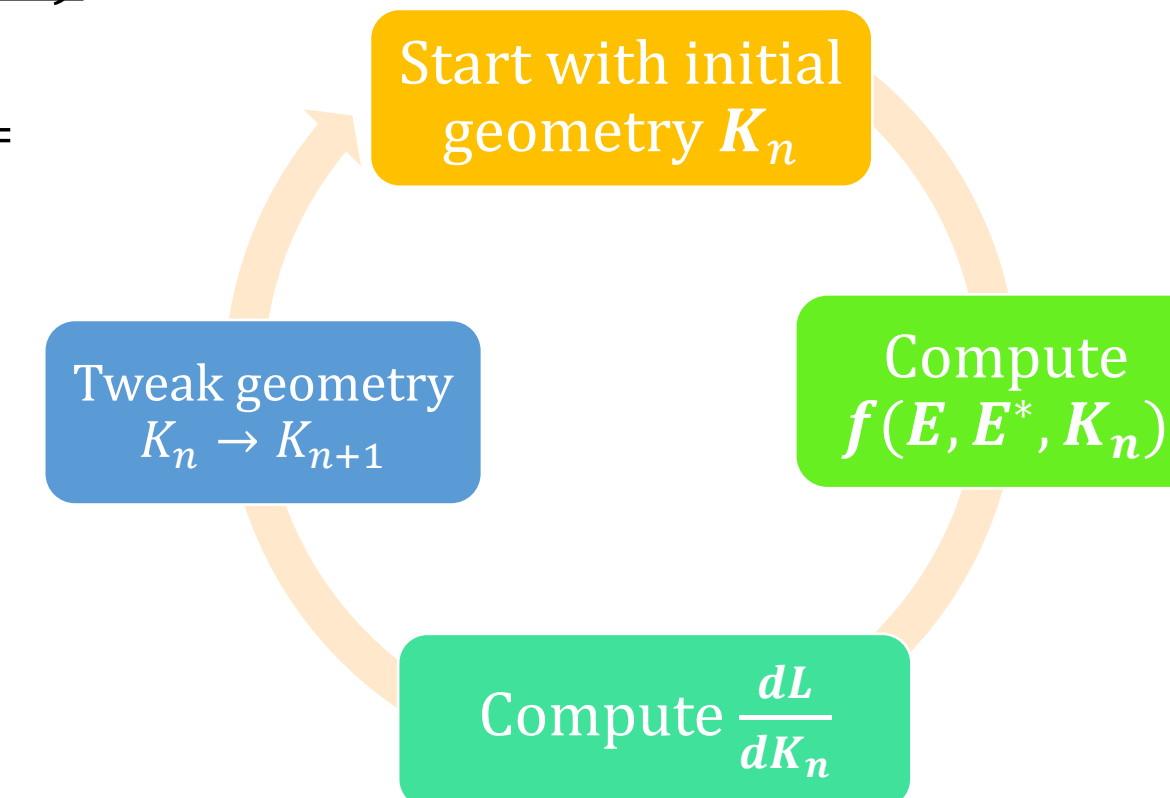
Optimize objective function $L(E, E^*, K)$

$$\begin{aligned} K &:= \text{vector of design variables} \\ E &\text{ is solution to } f(E, E^*, K) = A(\epsilon_r)E - b = \\ & \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) E + K^2(1 + \chi|E|^2)E - \text{src} = 0 \end{aligned}$$

Adjoint method computes gradient of objective w.r.t. design variables:

$$\frac{dL}{d\epsilon_r} = \frac{\partial L}{\partial \epsilon_r} - 2\omega_0^2 \epsilon_0 * \text{Re}(E_{adj}^T E)$$

Tweak design variables and re-compute $f(E, E^*, K)$



[2]

Computational Scheme

Discretize and flatten vector E:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) E + k^2 n^2 E - b = 0$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u + K^2 u - \text{src} = 0$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) u[p] + K[p]^2 u[p] - \text{src}[p] = 0$$

Solving inverse jacobian with Krylov Method (GMERS):

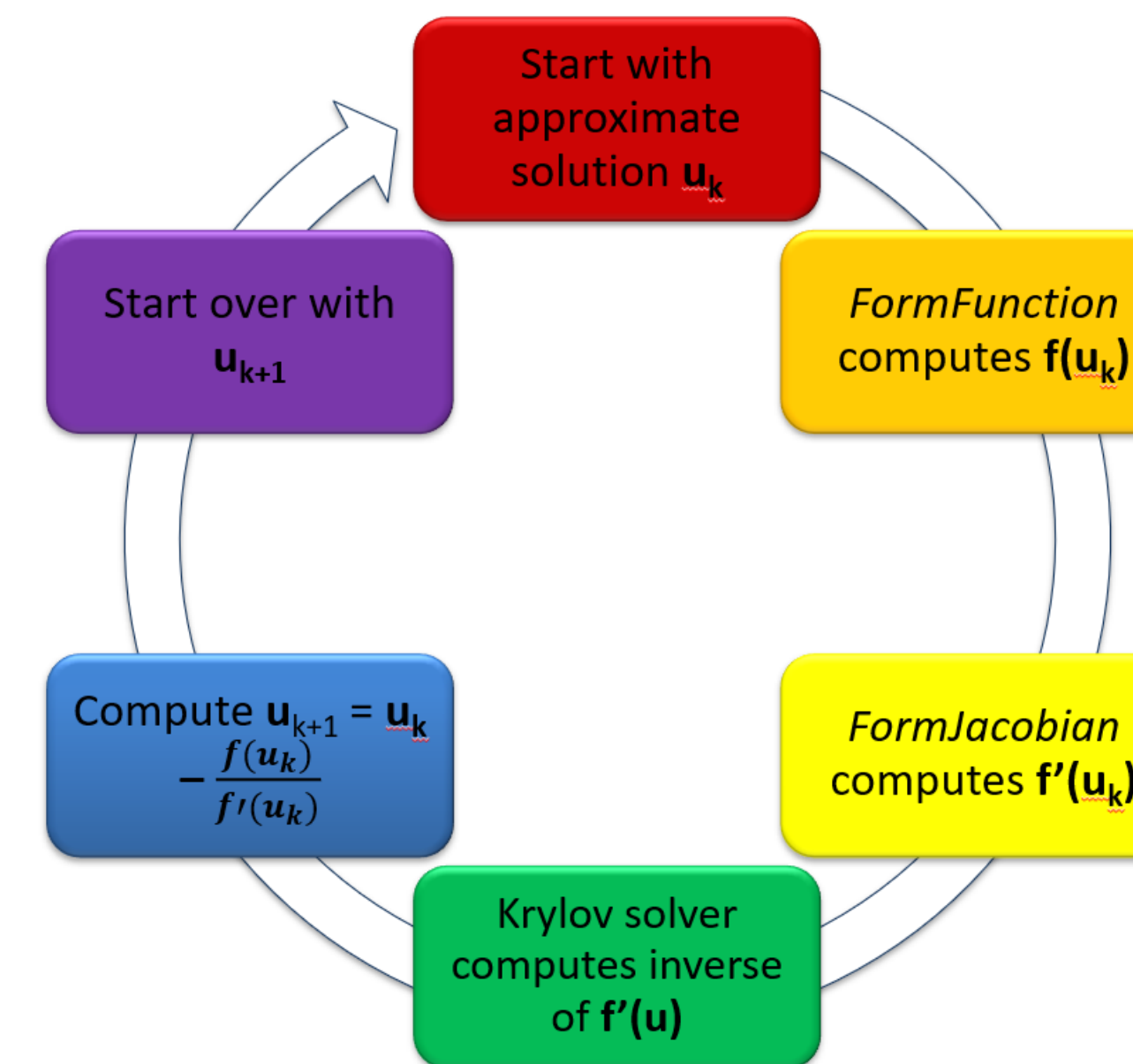
$$\begin{aligned} &\text{Conjugate Gradient Method} \\ &r_0 = b - Ax_0 \\ &p_0 = r_0 \\ &\text{for } k = 0, 1, 2, \dots \\ &\alpha_k = r_k^T r_k / p_k^T A p_k \\ &x_{k+1} = x_k + \alpha_k p_k \\ &r_{k+1} = r_k - \alpha_k A p_k \\ &\beta_{k+1} = r_{k+1}^T r_{k+1} / r_k^T r_k \\ &p_{k+1} = r_{k+1} + \beta_{k+1} p_k \\ &\text{end} \end{aligned}$$

Implement *FormFunction()* and *FormJacobian()* for use in **Newton's Method**:

For discretized function f and approximate solution u_k :

$$u_{k+1} = u_k - \frac{f(u_k)}{f'(u_k)}$$

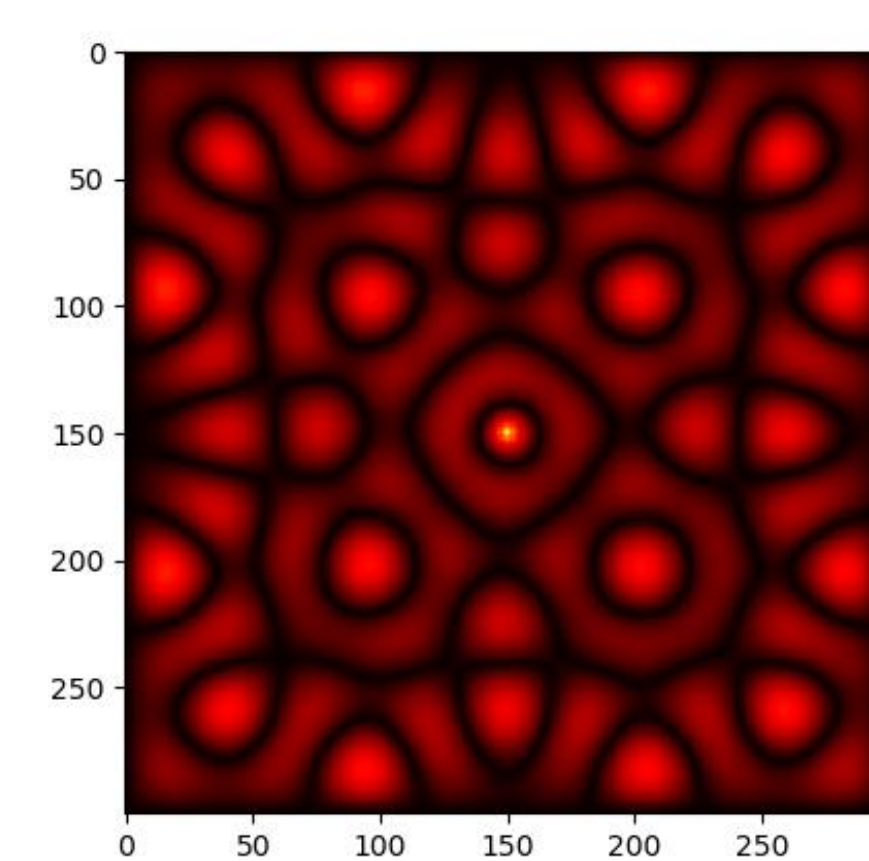
Where $\dim(f) = \dim(u) = n$ and $\dim(f'(u_k)) = n \times n$



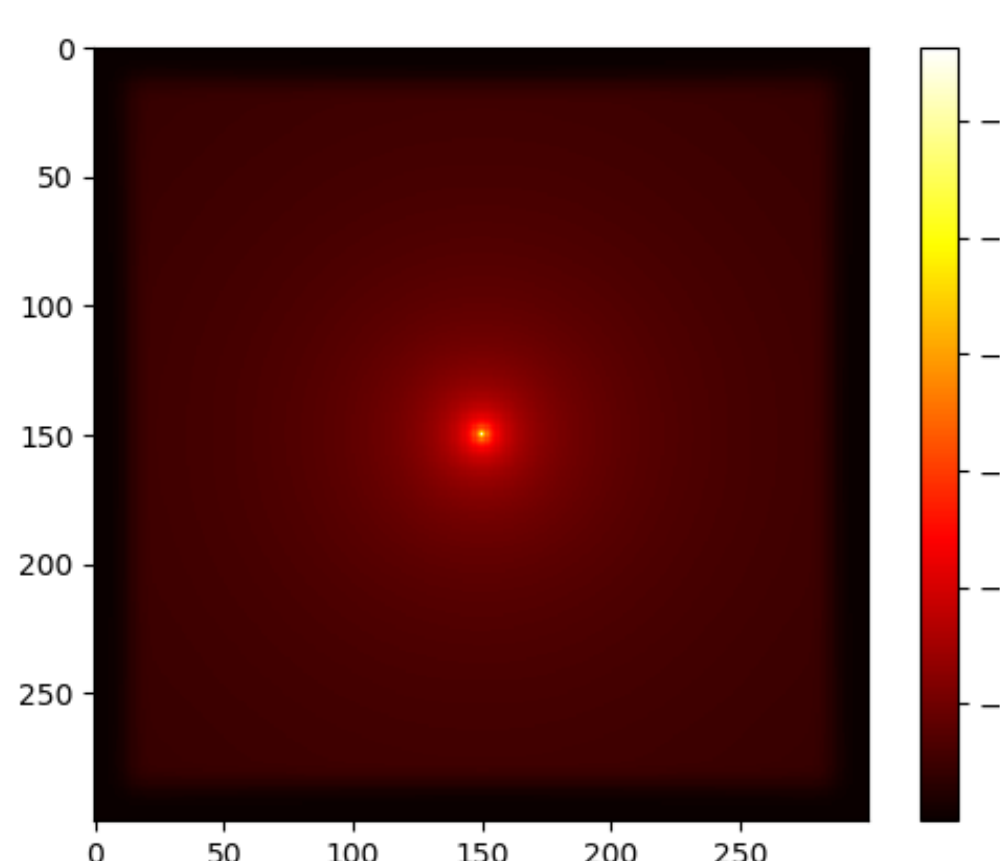
[3,4]

Perfectly Matched Layer

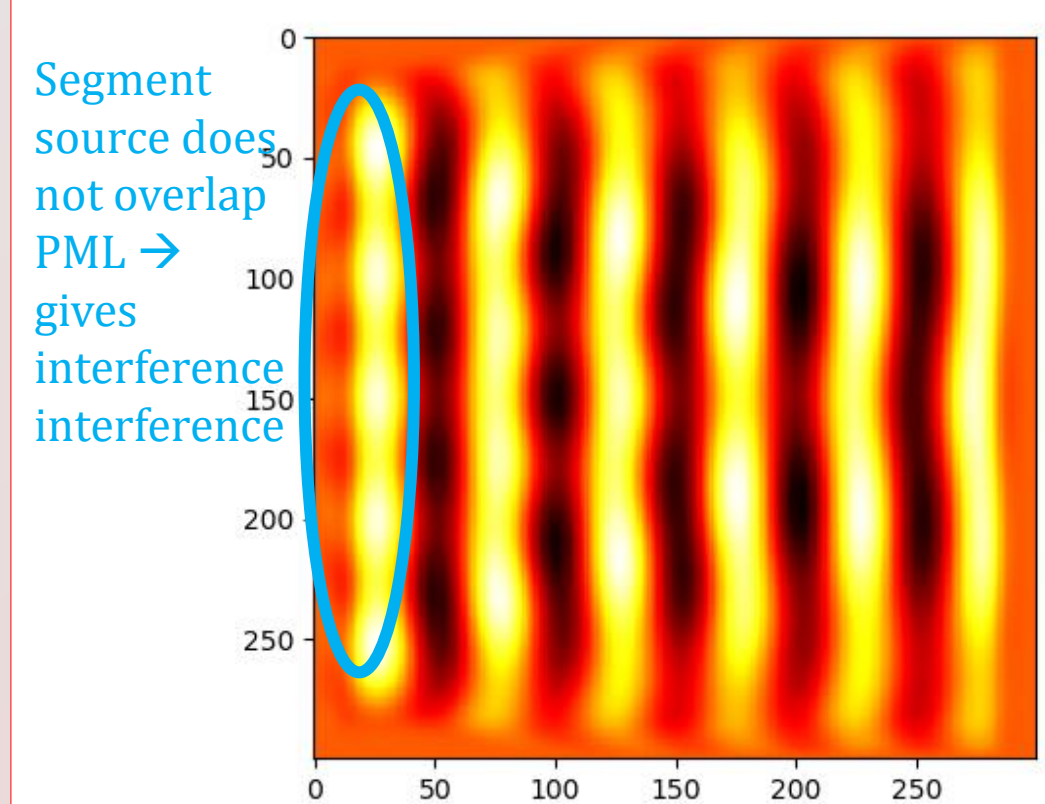
Enforcing hard-wall boundary condition gives reflections at the boundary:



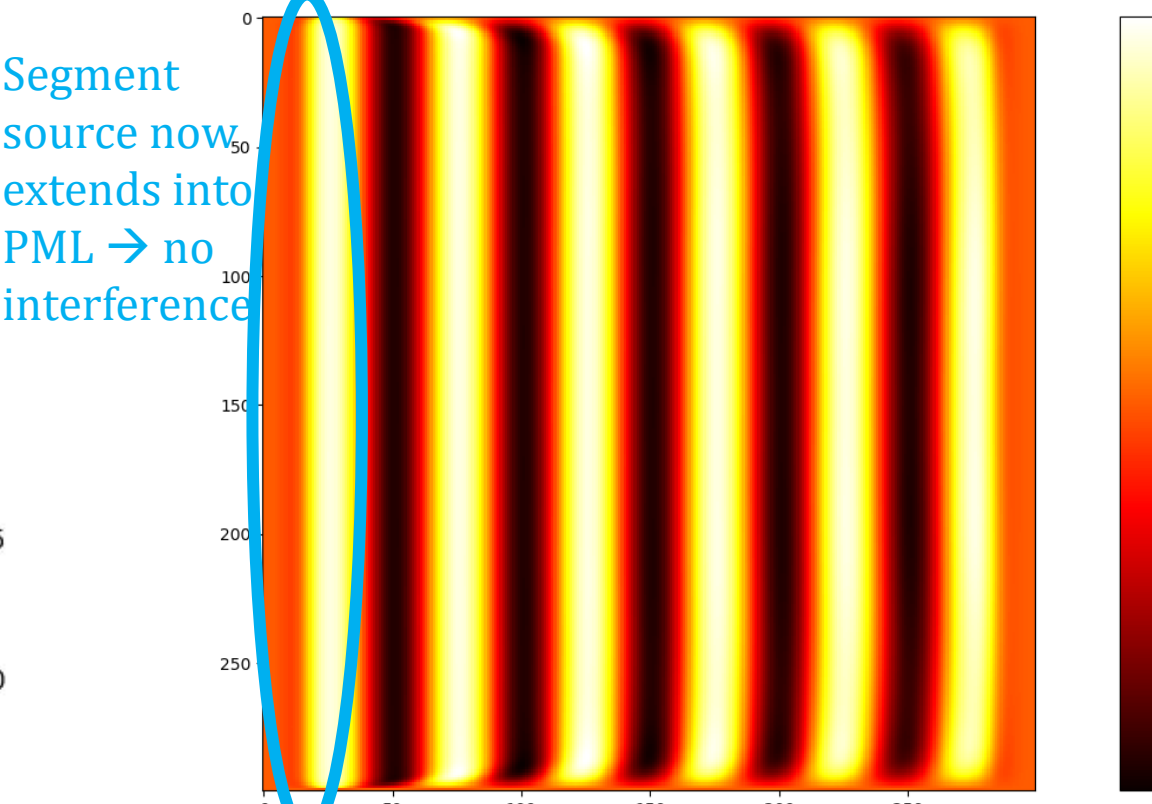
Perfectly Matched Layer (PML) exponentially attenuates waves near the border:



Also makes possible simulations of geometries that extend infinitely in any direction:

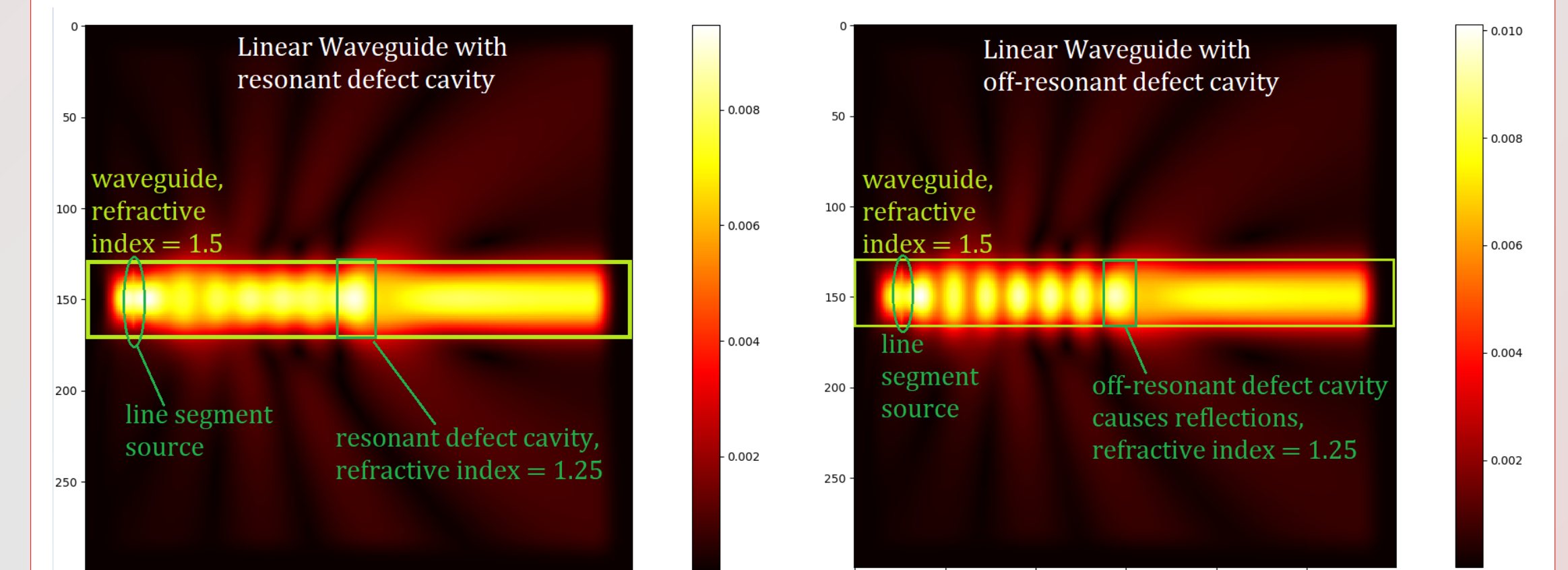


Accomplished through stretching near boundary: $\frac{\partial}{\partial x} \rightarrow \frac{1}{1 + i\sigma(x)/\omega} \frac{\partial}{\partial x}$

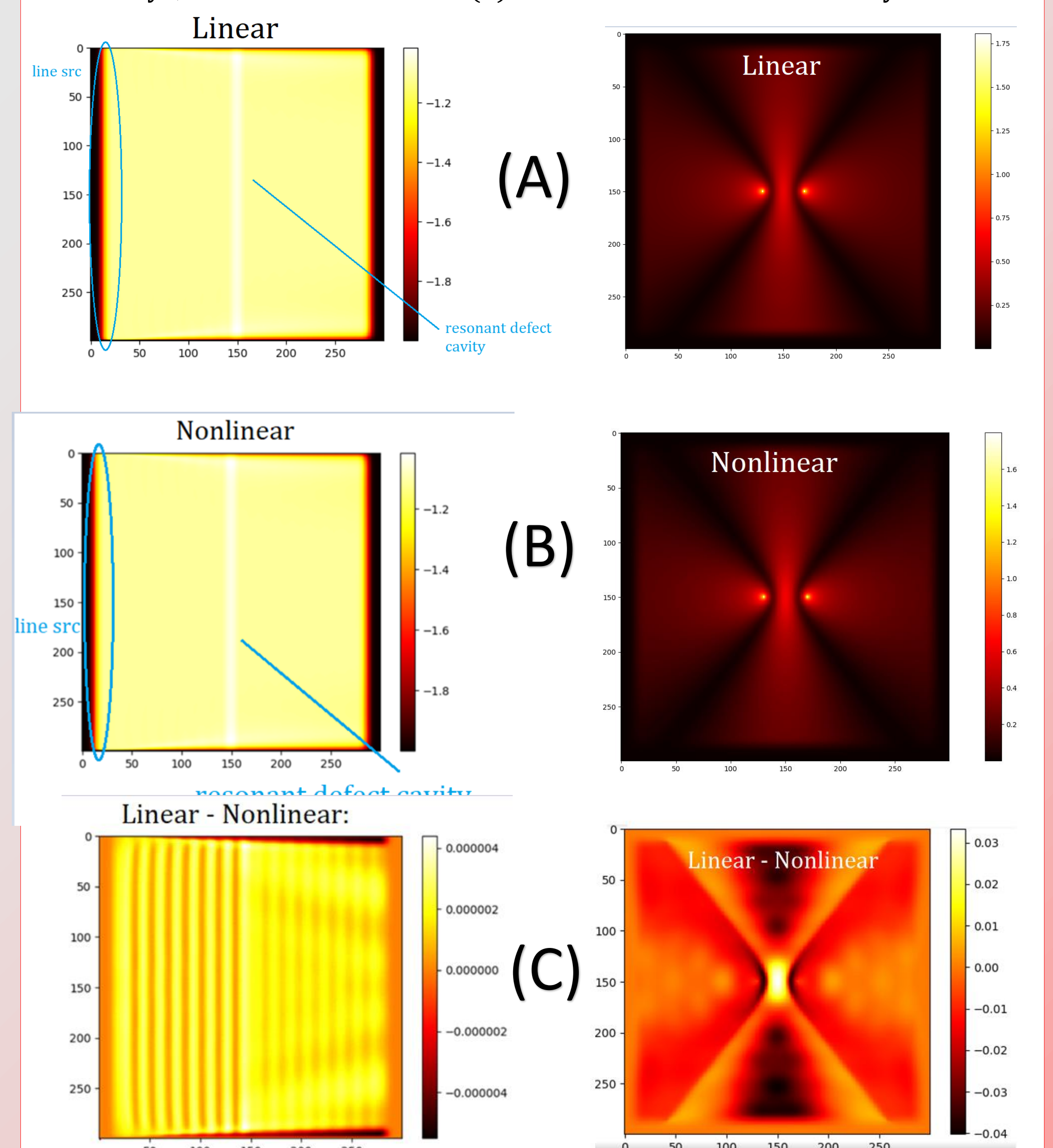


[5]

Examples



Linear version (A) has $\chi = 0$. linear and nonlinear (B) look identical to the naked eye; we take the difference (C) to see the effect of nonlinearity:



Conclusion

We are developing an inverse design computational scheme that will allow us to discover optical structures based on desired functional characteristics. Although our focus is on the design of broad-band efficient optical limiters the method can find application in a broader range of photonic devices. Its main strength is the fact that it opens up the possibility to exploit in an efficient manner an enlarge parameter space of available material knowledge and physical principles aiming to deliver devices with ultimate achievable performance.

References

1. J.H. Vella, et al, Experimental realization of a reflective optical limiter, Physical Review Applied 5.6 (2016): 064010.
2. S. Molesky, Z. Lin, A.Y. Piggott, et al, Inverse design in nanophotonics, Nature Photon 12, 659–670 (2018). <https://doi.org/10.1038/s41566-018-0246-9>
3. L. Dalcin, P. Kler, R. Paz, and A. Cosimo, Parallel Distributed Computing using Python, Advances in Water Resources, 34(9):1124-1139, (2011). <http://dx.doi.org/10.1016/j.advwatres.2011.04.013>
4. S. Balay, S. Abhyankar, M. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, A. Dener, V. Eijkhout, W. Gropp, D. Karpeyev, D. Kaushik, M. Knepley, D. May, L. Curfman McInnes, R. Mills, T. Munson, K. Rupp, P. Sanan, B. Smith, S. Zampini, H. Zhang, and H. Zhang, PETSc Users Manual, ANL-95/11 - Revision 3.13, (2020). <http://www.mcs.anl.gov/petsc/petsc-current/docs/manual.pdf>
5. J. Fang and Z. Wu, Generalized perfectly matched layer for the absorption of propagating and evanescent waves in lossless and lossy media, in IEEE Transactions on Microwave Theory and Techniques, vol. 44, no. 12, pp. 2216-2222, Dec. (1996), doi: 10.1109/22.556449.