When PML isn't P:

Limitations of Perfectly Matched Layers

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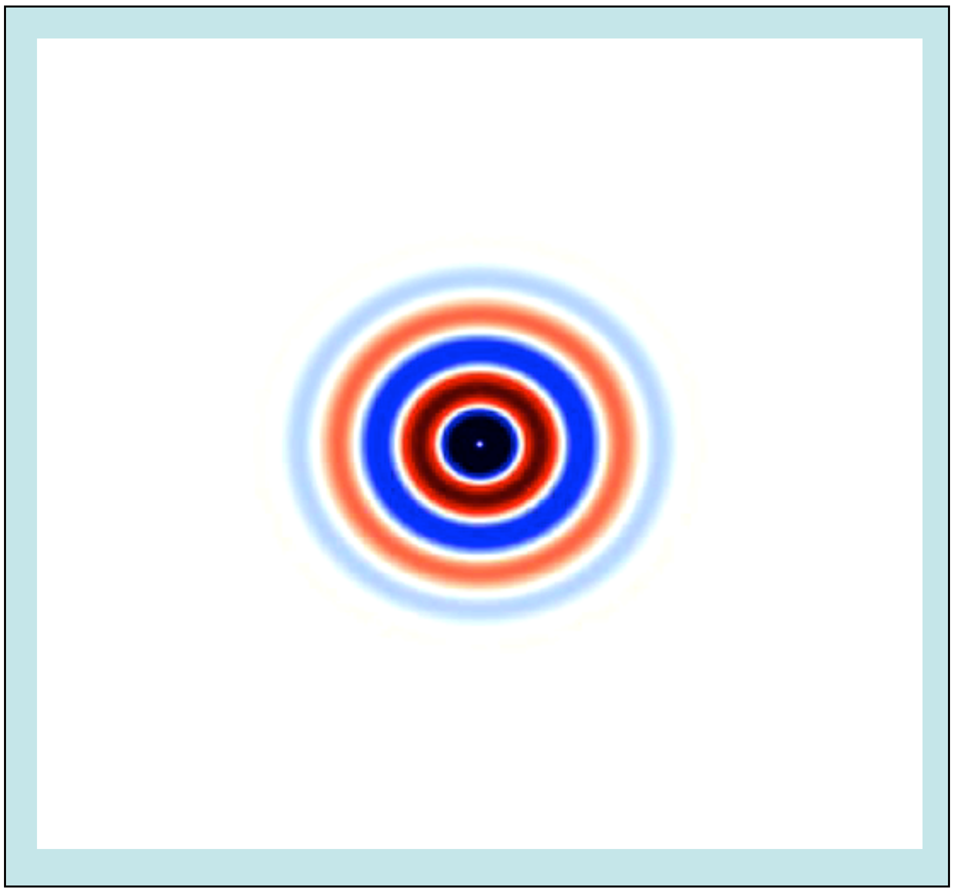
Why Absorbers?

Finite-difference/finite-element volume discretizations need to artificially truncate space for a computer simulation.



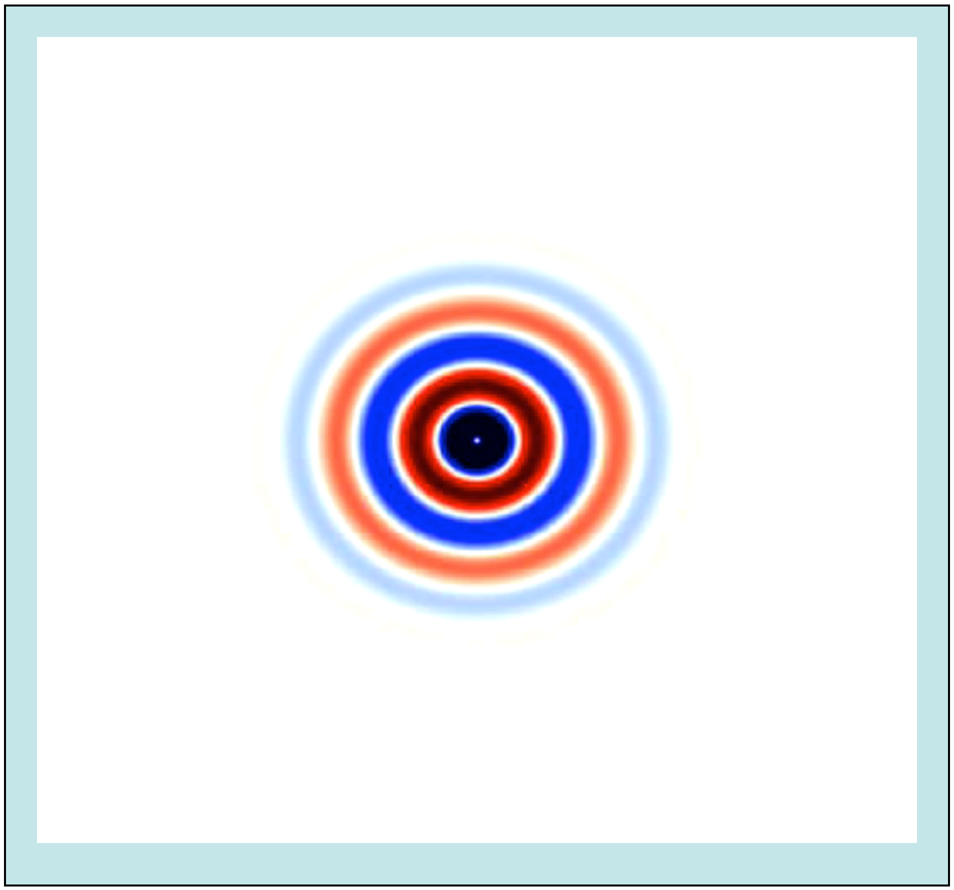
In a wave equation, a hard-wall truncation gives reflection artifacts.

An old goal: "absorbing boundary condition" (ABC) that absorbs outgoing waves.

Problem: good ABCs are hard to find in > 1d.

Absorbing Boundary *Layers*?

…instead of absorbing boundary *condition*,
make an absorbing *layer* that attenuates waves…



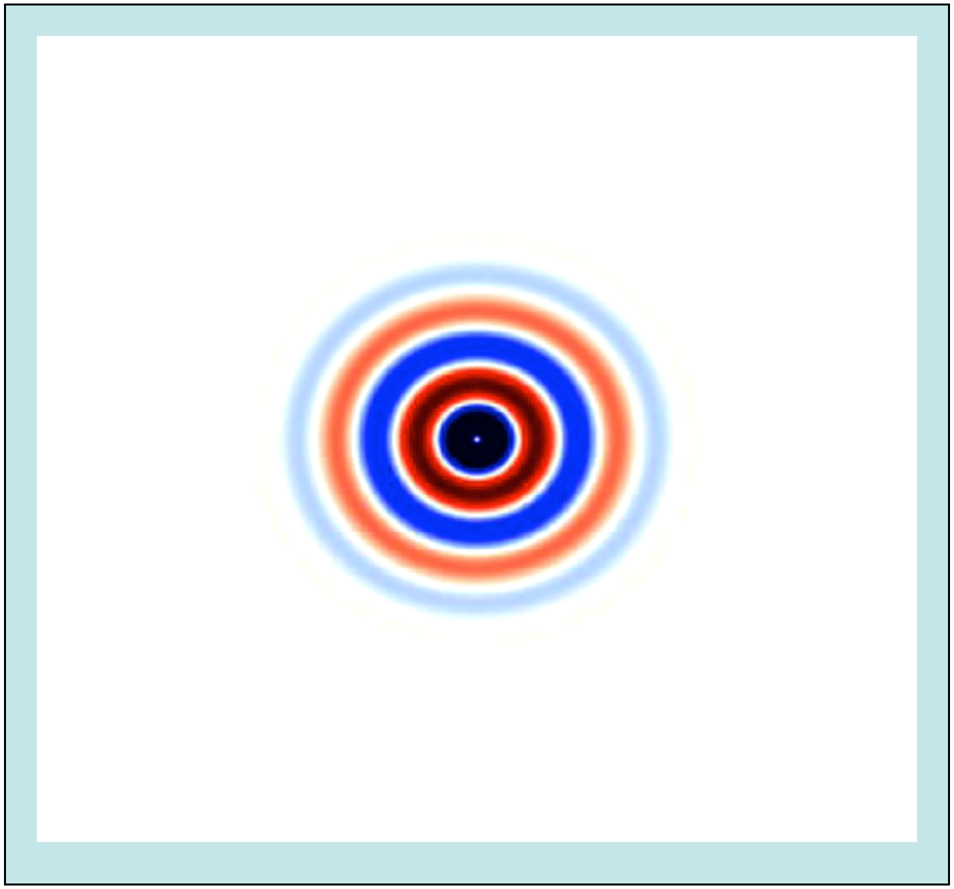
Simplistic approach:

Just put some conductivity σ around the boundaries?

Problem: reflections at interface of absorbing region

Absorbing Boundary *Layers*?

…instead of absorbing boundary *condition*,
make an absorbing *layer* that attenuates waves…



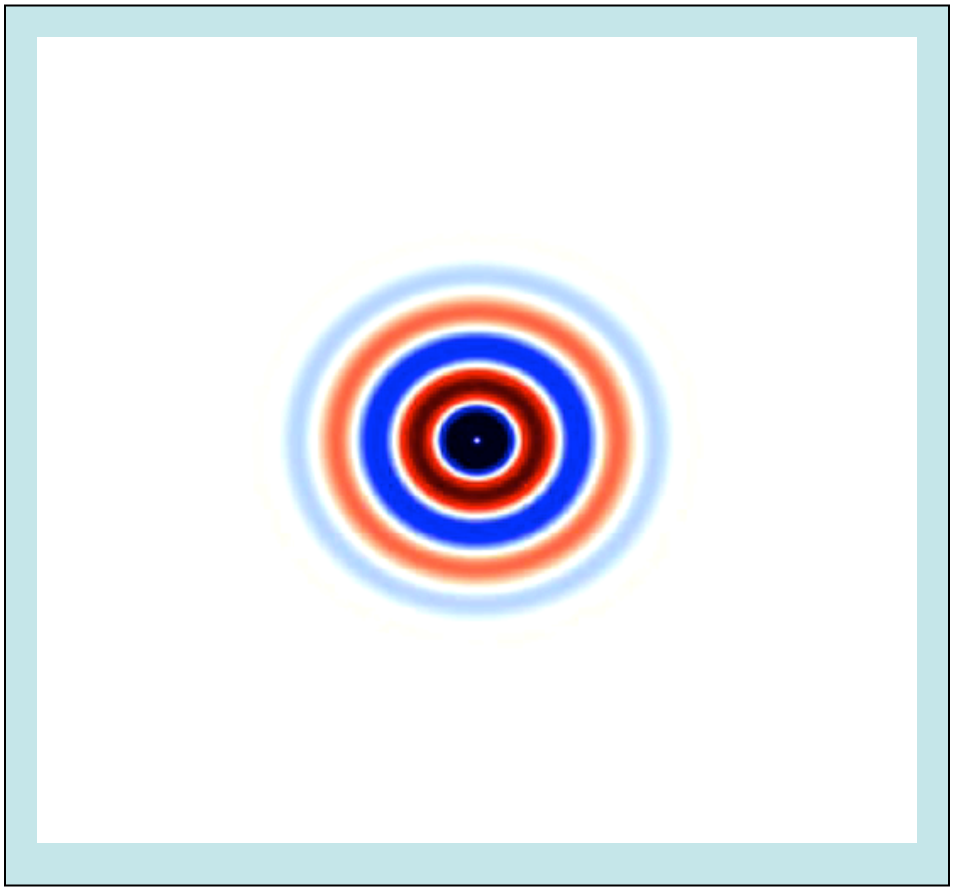
Less simplistic approach:

Conductivity σ by boundaries turns on gradually to reduce reflections — e.g., quadratically

Better, but visible reflections w/o very thick/gradual absorber

Perfectly Matched Layers (PMLs)

Bérenger, 1994: design an *artificial* absorbing layer
that is analytically reflectionless



Works *remarkably well*.

Now ubiquitous in FD/FEM wave-equation solvers.

(Here, I'll mainly discuss the example of Maxwell's eq.)

Perfectly Matched Layers (PMLs)

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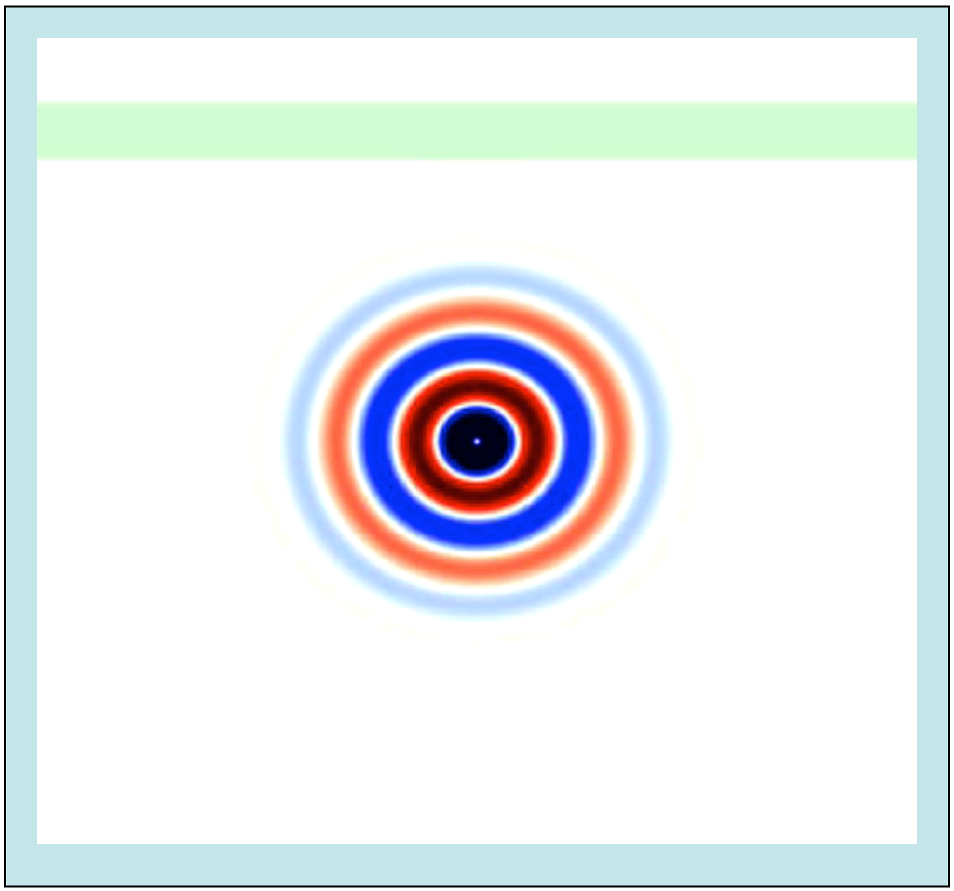

Even works in inhomogeneous media (e.g. waveguides).

Two questions:

- *Review:* How does PML work?
- When does PML *not* work?

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- *Review:* How does PML work?
- When does PML *not* work?

Three equivalent approaches

- Bérenger (1994): design artificial equations ("split fields")
  so that planewaves in vacuum are reflectionless
- Sacks et al. (1995): design artificial materials (anisotropic ε, μ)
  so that planewaves in vacuum are reflectionless

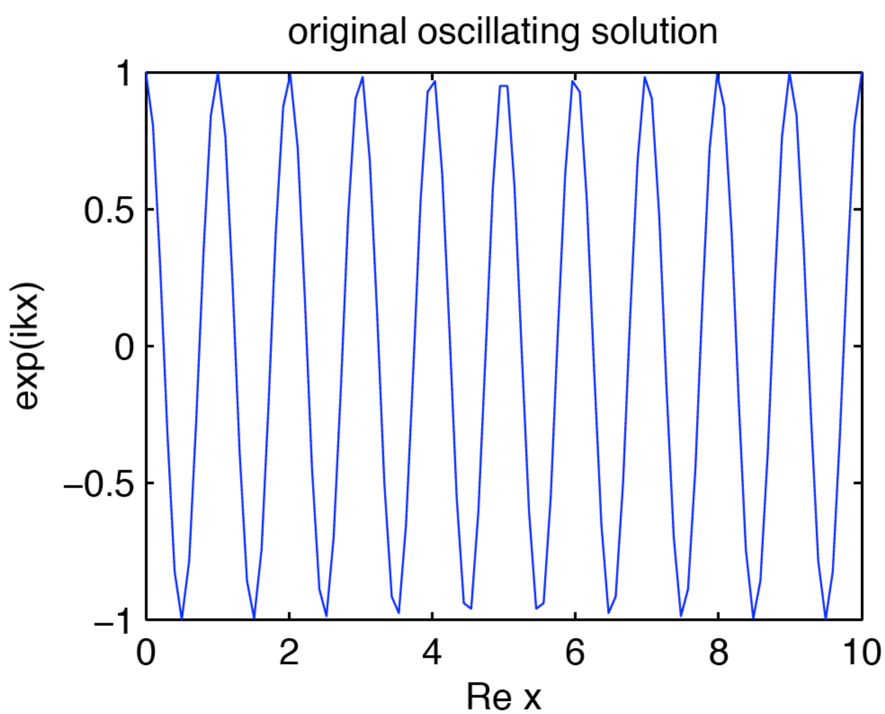
- Chew & Weedon (1994): complex coordinate "stretching"
  so that waves in *any*(?) medium are attenuated.

… Ward & Pendry (1996): coordinate transformations are
equivalent to transformed/anisotropic ε, μ
… leads back to artificial materials (Teixeira & Chew, 1998)

Starting point: A propagating wave

- Say we want to absorb wave traveling in $+x$ direction in an x-invariant medium at a frequency $\omega > 0$.

$$\text{fields} \sim f(y,z)e^{i(kx-\omega t)} \qquad (usually, k > 0)$$



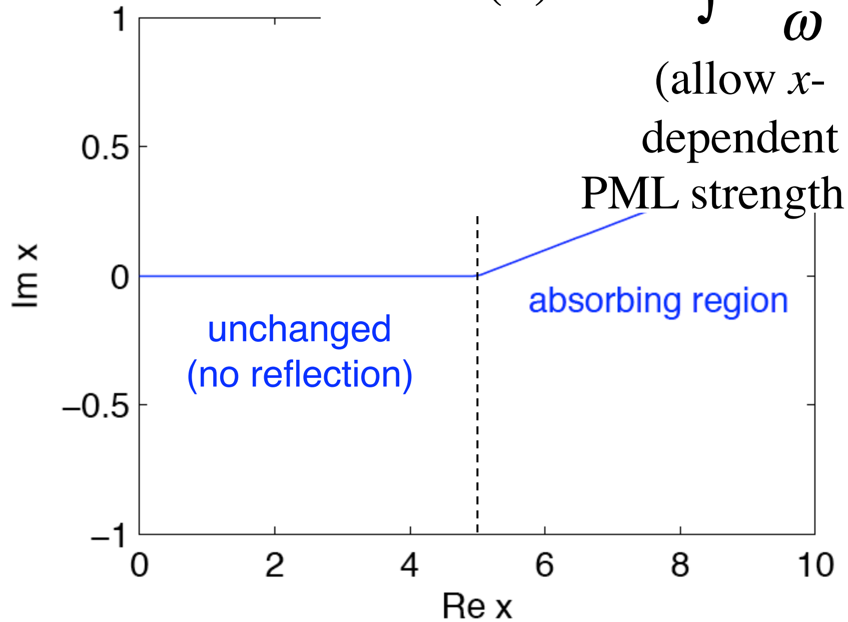
(only x in wave equation is via $\partial / \partial x$ terms.)

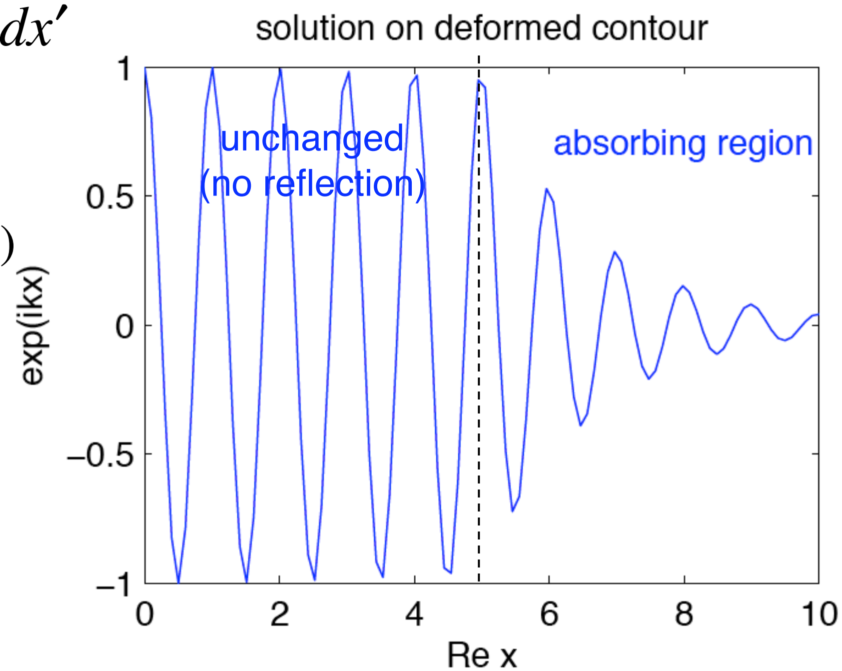
Step 1: Analytically continue

Fields (& wave equation terms) are *analytic* in x,
so we can evaluate at complex x & still solve same equations

$$\tilde{x}(x) = x + \int^{x} \frac{i\sigma(x')}{\omega} dx'$$

(allow x-dependent PML strength σ)





$$\text{fields} \sim f(y,z)e^{i(kx-\omega t)} \to f(y,z)e^{i(kx-\omega t)-\frac{k}{\omega}\sigma x}$$

Step 2: Coordinate transformation

Weird to solve equations for complex coordinates $\tilde{x}$,
so do coordinate transformation back to real x.

$$\tilde{x}(x) = x + \int^{x} \frac{i\sigma(x')}{\omega} dx'$$

(allow x-dependent PML strength σ)

$$\frac{\partial}{\partial x} \overset{①}{\rightarrow} \frac{\partial}{\partial \tilde{x}} \overset{②}{\rightarrow} \left[\frac{1}{1 + \frac{i\sigma(x)}{\omega}} \right] \frac{\partial}{\partial x}$$

$$\text{fields} \sim f(y,z) e^{i(kx - \omega t)} \rightarrow f(y,z) e^{i(kx-\omega t) - \frac{k}{\omega}\int^{x} \sigma(x')\, dx'}$$

nondispersive materials: $k/\omega \sim$ constant
⇒ decay rate independent of ω

Step 3: Effective materials

In Maxwell's equations, $\nabla \times \mathbf{E} = i\omega\mu\mathbf{H}, \quad \nabla \times \mathbf{H} = -i\omega\varepsilon\mathbf{E} + \mathbf{J}$,
coordinate transformations are *equivalent* to transformed *materials*
(Ward & Pendry, 1996: "transformational optics")

$$\{\varepsilon, \mu\} \to \frac{J\{\varepsilon, \mu\}J^T}{\det J}$$

x PML Jacobian

$$J = \begin{pmatrix} (1+i\sigma/\omega)^{-1} & & \\ & 1 & \\ & & 1 \end{pmatrix}$$

$$\left(\frac{\partial x}{\partial \tilde{x}}\right)$$

for isotropic starting materials:

$$\{\varepsilon, \mu\} \to \{\varepsilon, \mu\} \begin{pmatrix} (1+i\sigma/\omega)^{-1} & & \\ & 1+i\sigma/\omega & \\ & & 1+i\sigma/\omega \end{pmatrix}$$

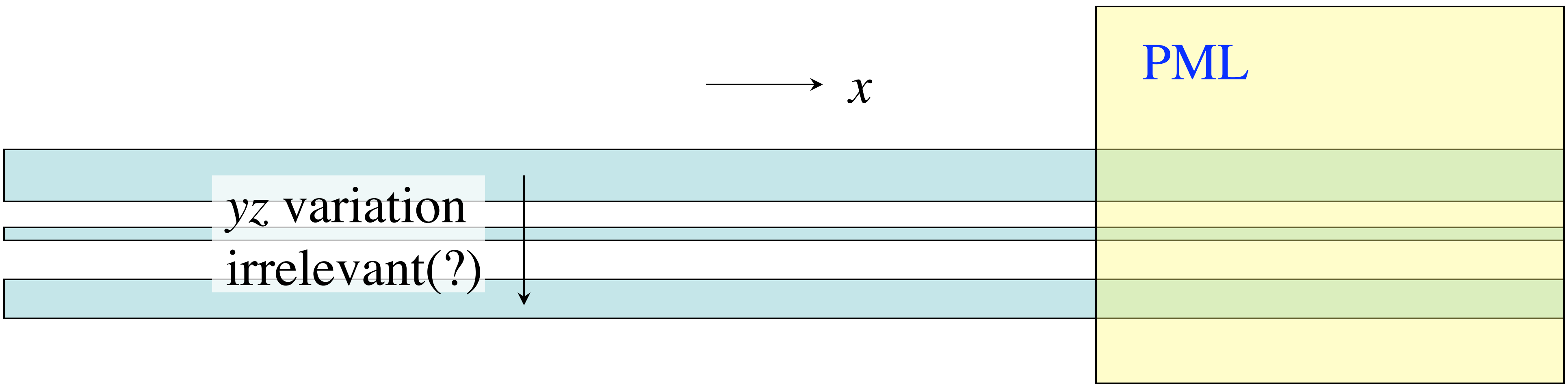
effective conductivity

PML = effective anisotropic "absorbing" ε, μ

PML Magic

$$\{\varepsilon,\mu\} \rightarrow \{\varepsilon,\mu\}\begin{pmatrix} (1+i\sigma/\omega)^{-1} & & \\ & 1+i\sigma/\omega & \\ & & 1+i\sigma/\omega \end{pmatrix}$$

sprinkle the "magic PML dust" onto your materials, and they become absorbing without reflections…



Two questions:

- *Review:* How does PML work?
- When does PML *not* work?

x-varying media

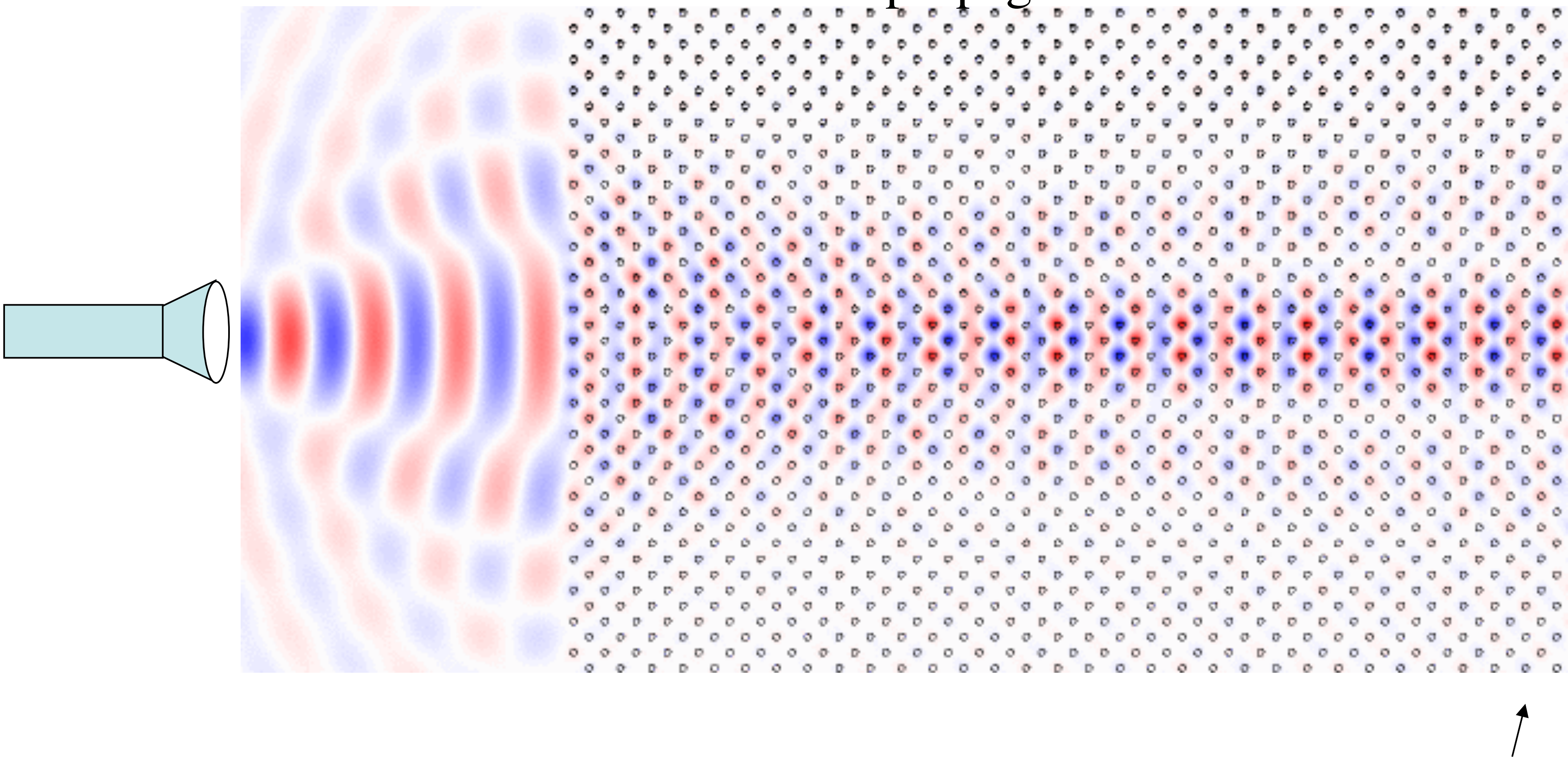
What happens if medium is varying in the x direction (i.e., $\perp$ to PML)?

Who cares?

— If it's x-varying, surely propagating waves scatter anyway … absorbers are irrelevant?

The magic of periodicity

coherent propagation: Bloch wave

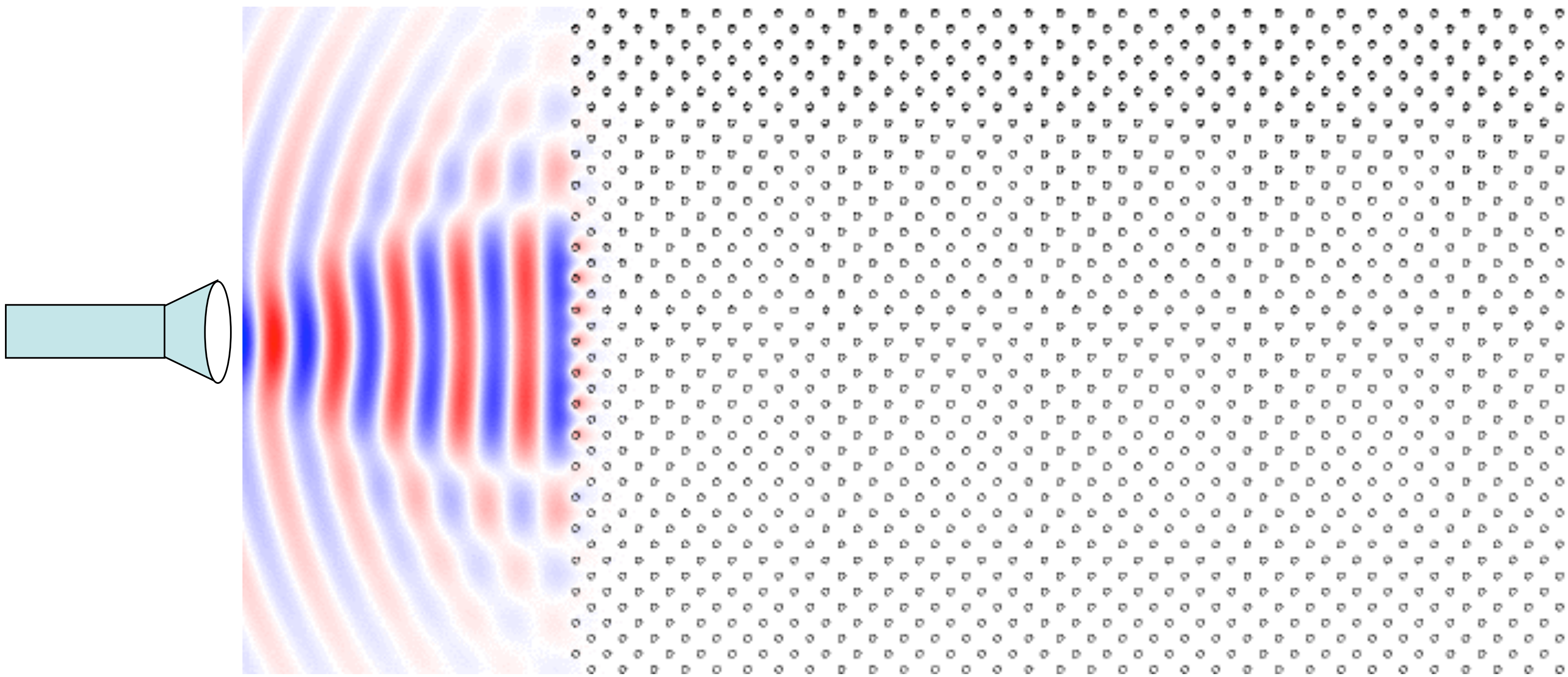


absorbing layer?

Light in a periodic medium (= photonic crystal) can propagate without scattering

A slight change? Shrink λ by 20%

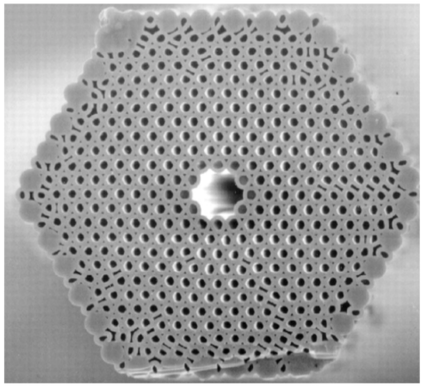
an "optical insulator" (photonic bandgap)



light cannot penetrate the structure at this wavelength!

all of the scattering destructively interferes

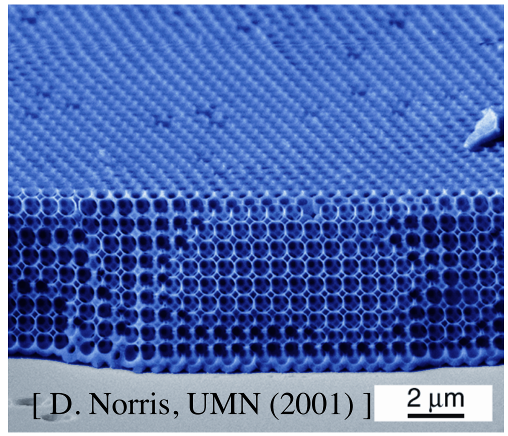
Photonic crystals: Periodic EM media



trapping/guiding light in vacuum

[Cregan (1999)]

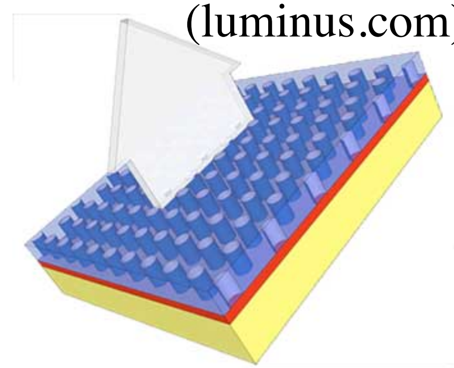
optical "insulators"



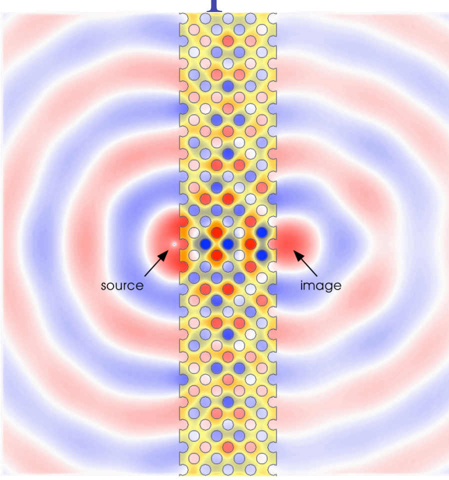
[D. Norris, UMN (2001)]

ultra-bright LEDs

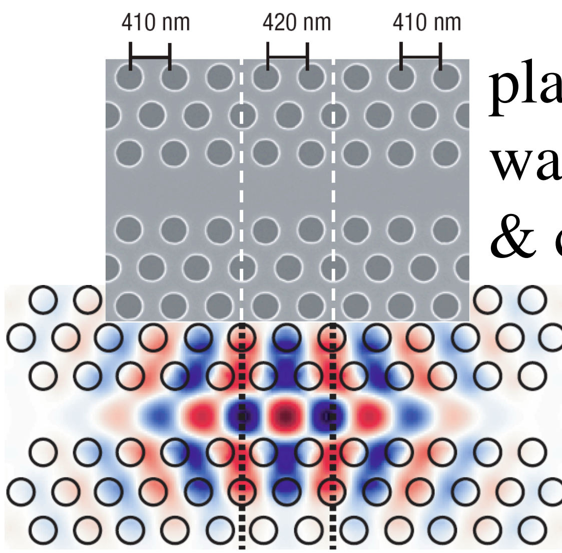
(luminus.com)



flat "superlenses"

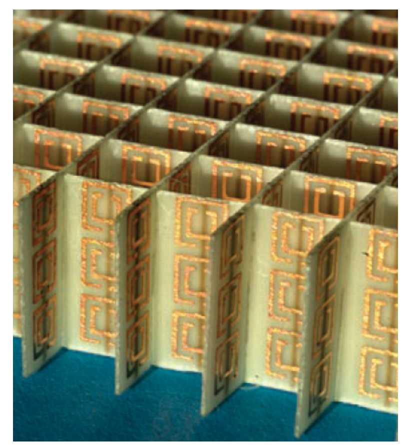


[Luo (2003)]



planar waveguides & cavities

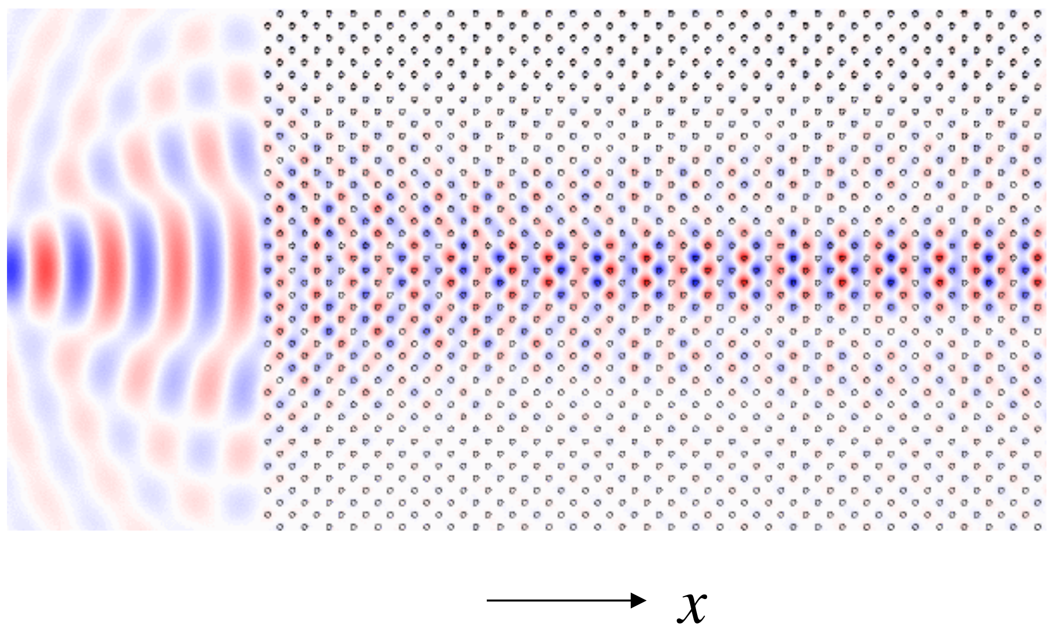
[Song (2005)]



metamaterials

[Smith (2004)]

Photonic-crystal PML?

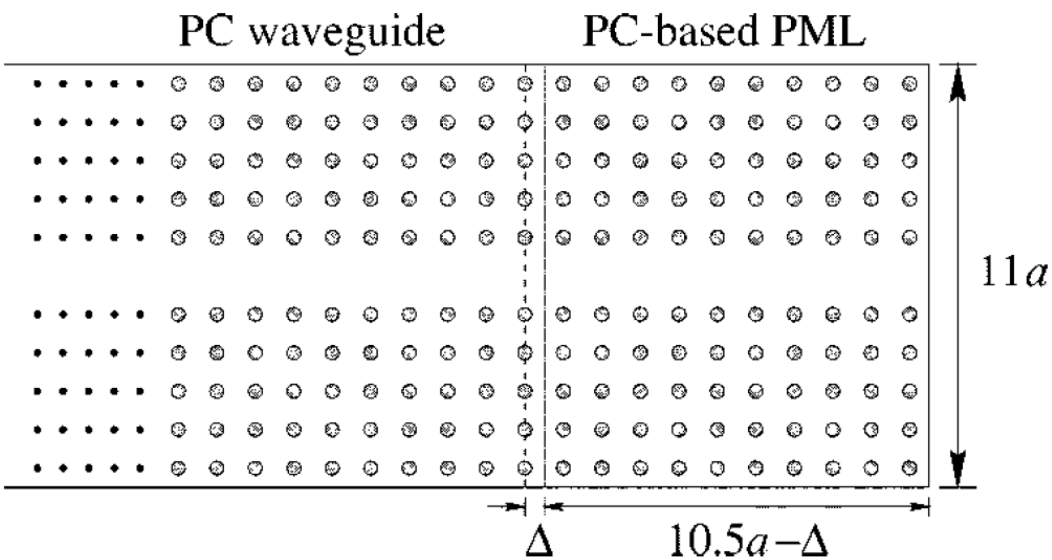


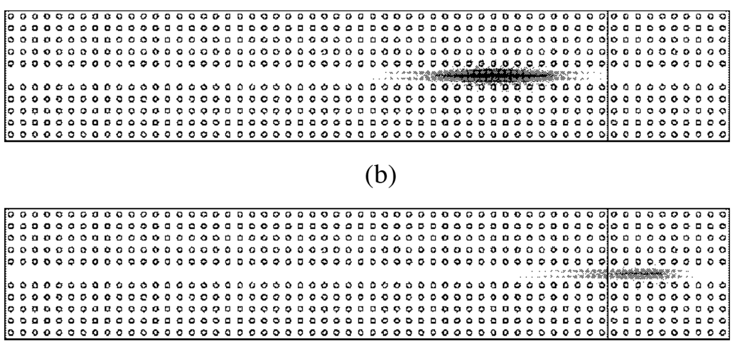
ε not even *continuous*
in x direction,
much less analytic!

Analytic continuation of Maxwell's equations is hopeless
— no reason to think that PML technique should work

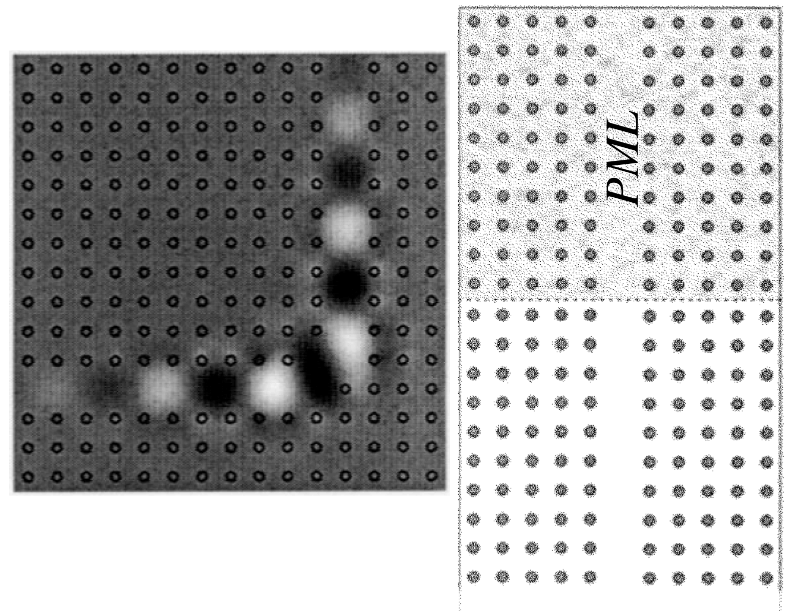
Photonic-crystal PMLs: Magic dust?

[Koshiba, Tsuji, & Sasaki (2001)]





[Kosmidou *et al* (2003)]



… & several other authors …

Low reflections claimed

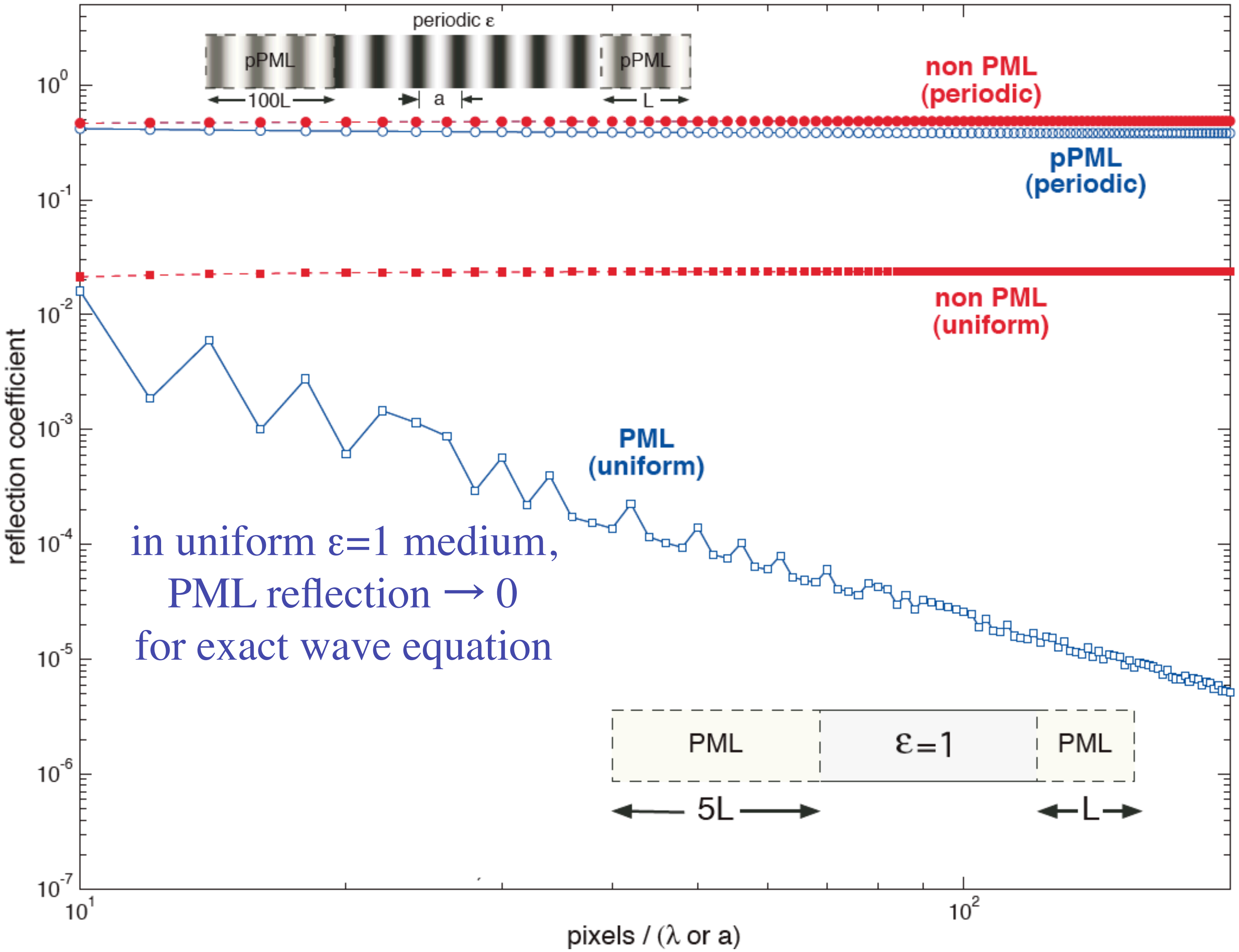
— is PML working?

Something suspicious:

very thick absorbers.

Failure of Photonic-crystal "pseudo-PML"

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]



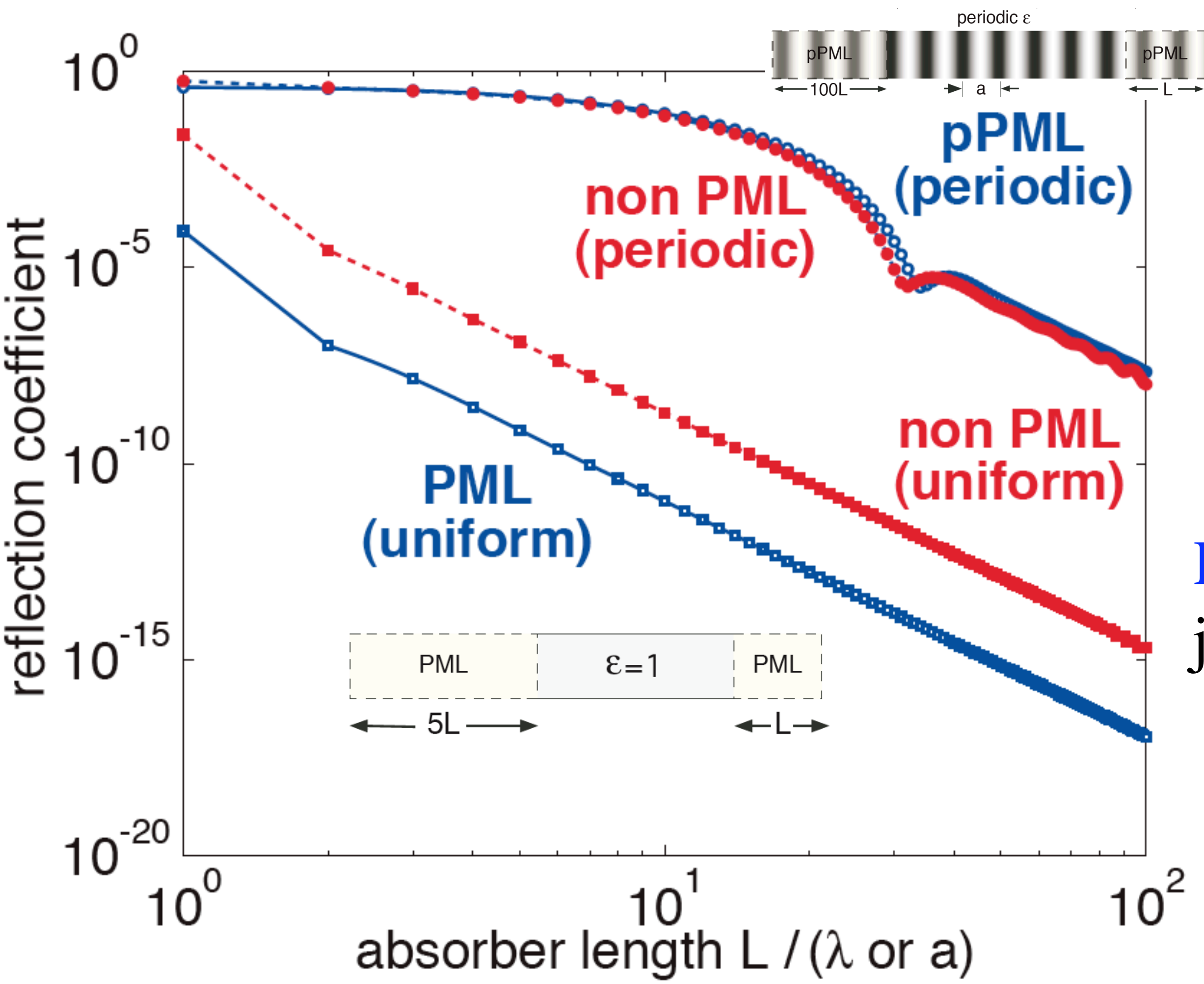
1d test case:

(pseudo-) PML in periodic ε reflection doesn't → 0 as $\Delta x \to 0$

… similar to non-PML scalar σ

Redemption of the pseudo-PML: *slow (adiabatic) absorption turn-on*

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]

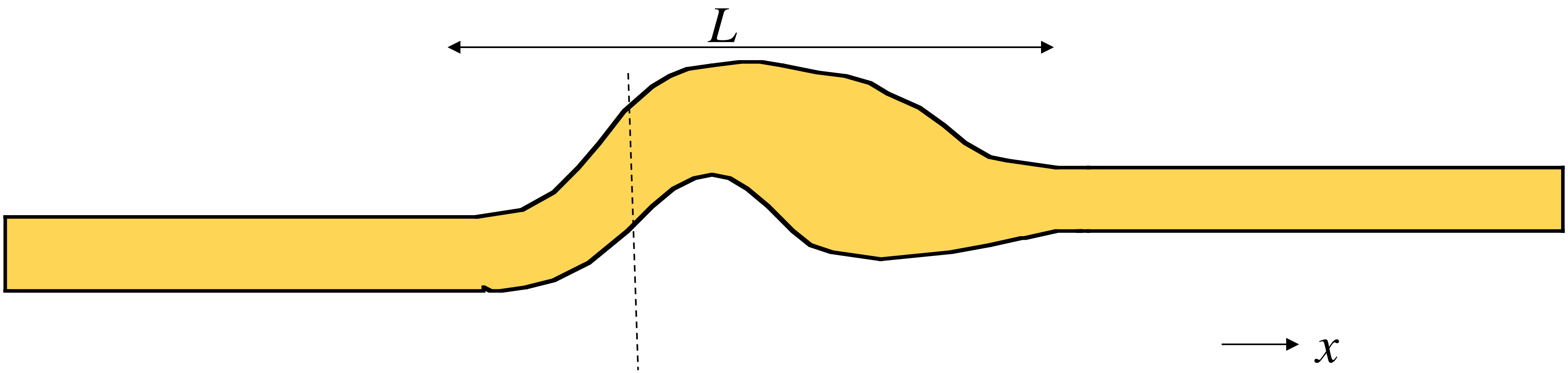


Any absorber, turned on gradually enough, will have reflections → 0!

PML (when it works) just helps coefficient.

Understanding gradual change: Coupled-wave theory

[basic idea dates back to 1950s & earlier]



expand fields in eigenmodes ψ_n of each cross-section:

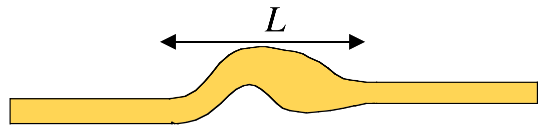
$$\text{fields}(x) = \sum_n c_n(x)\,\psi_n(y,z)\,e^{-i\omega t + i\int^x k_n(x')\,dx'}$$

→ ODEs for $c_n(x)$

[non-trivial extension to periodic media: Johnson (2002)]

Coupled-mode equations

- Rescale $u = x/L$



- Parameterize structure by $s(u)$: $[0,1] \rightarrow [0,1]$

$$\frac{dc_m}{du} = \sum_{n \neq m} s'(u) \frac{M_{nm}[s(u)]}{\Delta k_{nm}[s(u)]} e^{iL\int^{u} \Delta k_{nm}[s(u')]\,du'} c_n(u)$$

rate of change

matrix element

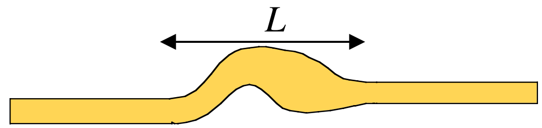
phase mismatch

Limit of large L (gradual taper):

$c_n(u) \rightarrow c_n(0)$ "adiabatic theorem"

Lowest-order reflection

- Rescale $u = x/L$
- Parameterize structure by $s(u)$: [0,1] → [0,1]



$$c_{\text{reflected}}(L) = c_{\text{incident}} \int_0^1 s'(u) \frac{M_{nm}[s(u)]}{\Delta k_{nm}[s(u)]} e^{iL\int^u \Delta k_{nm}[s(u')]\,du'} du$$

say Δk real, definite-sign … change variables $\xi(u) = \int^u \Delta k_{nm}[s(u')]\,du'$

$$c_{\text{reflected}}(L) = c_{\text{incident}} \int_0^{\xi(1)} s'(u(\xi)) f(\xi) e^{iL\xi}\, d\xi$$

Fourier transform! Convergence → 0 depends on smoothness of $s'(u)$.

Back to absorption tapers

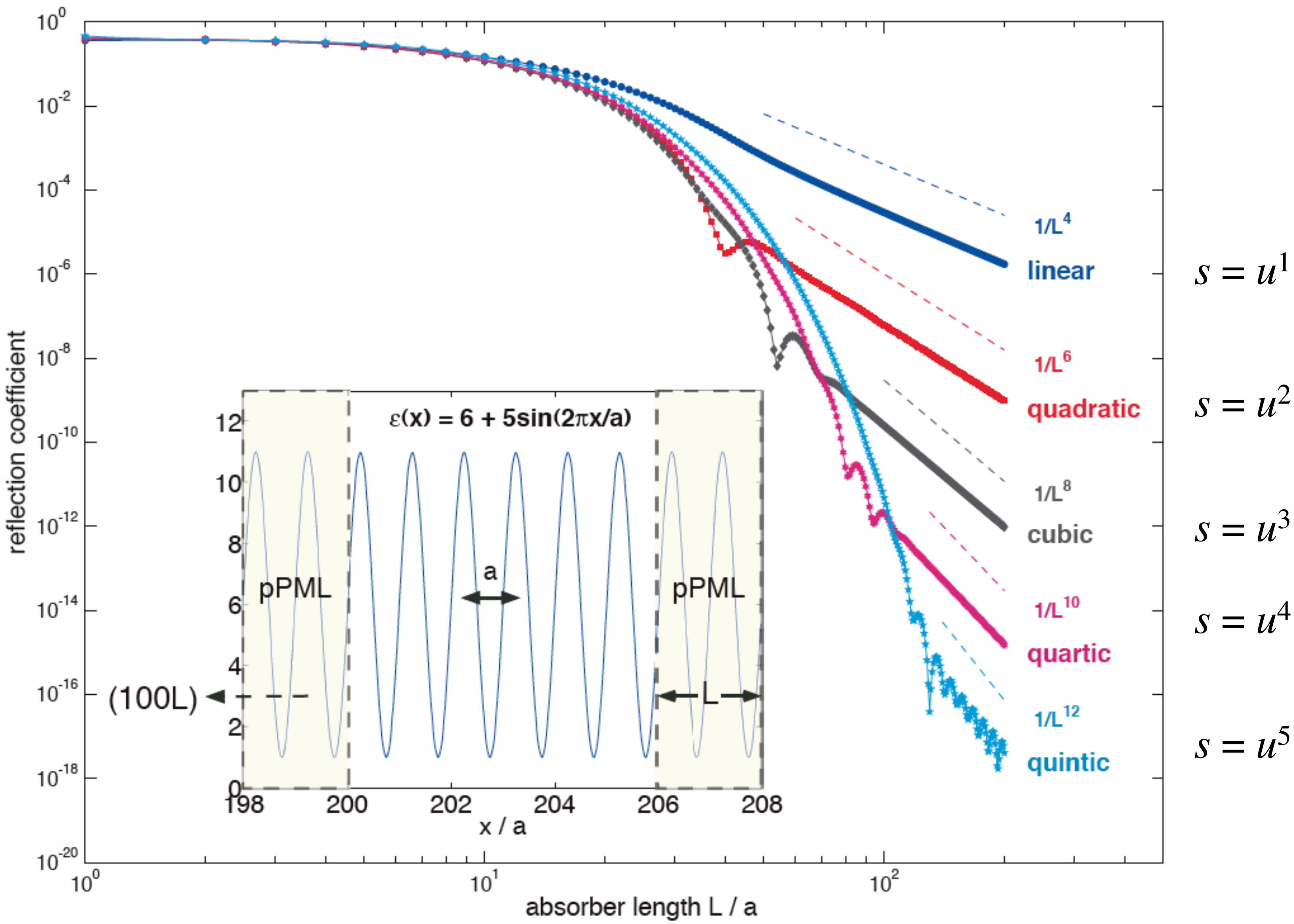
- Suppose absorption is: $\sigma(x) = \sigma_0\, s(x/L)$, say $s(u) = u^d$
- Fix the round-trip reflection: $R_{\text{round-trip}} = e^{-\#\, L\sigma_0 \int_0^1 s(u)\,du} \Rightarrow \sigma_0 \sim \frac{1}{L}$

$\Rightarrow \ldots \Rightarrow$ transition reflections $\sim O(L^{-2d-2})$

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]

Reflection vs. Absorber Thickness

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]



Adiabatic Absorbers: Parting Thoughts

- Turning on σ gradually is the backup plan when PML fails.
- Even real PML turns on σ gradually to mitigate discretization.
- Several reports of "working" PML in the literature turn out to be just adiabaticity.

- As the absorber length L becomes longer, smoother σ is beneficial.
  (exponential convergence is possible for C_∞ functions σ
  … but hard to get good constant factor)
- Finding the best adiabatic σ is a difficult problem
  — highly problem-dependent
  — but desirable to avoid thick absorbers, especially in 3d
  — min. L rapidly increase for "slow-light" (low v_g) systems

[Oskooi *et al*, *Optics Express* **16**, 11376 (2008)]

Two questions:

- *Review:* How does PML work?
- When does PML *not* work?

Starting point: A propagating wave

- Say we want to absorb wave traveling in $+x$ direction in an x-invariant medium at a frequency $\omega > 0$.

$$\text{fields} \sim f(y,z)e^{i(kx-\omega t)} \qquad (\textit{usually}, k > 0)$$

What if $k < 0$? i.e. $v_g = \mathrm{d}\omega/\mathrm{d}k > 0$ and $v_p = \omega/k < 0$?

PML: $$\text{fields} \sim f(y,z)e^{i(kx-\omega t)} \to f(y,z)e^{i(kx-\omega t)-\frac{k}{\omega}\sigma x}$$

Exponentially *growing* PML fields for $\sigma > 0$!!

Backward-Wave Modes?

$v_g = \mathrm{d}\omega/\mathrm{d}k > 0$ and $v_p = \omega/k < 0$

(in x-invariant media)

- Impossible in homogeneous media with $\varepsilon > 0$, $\mu > 0$
- Impossible in index-guided (total internal reflection) waveguides with $\varepsilon > 0$ [Bamberger & Bonnet (1990)]

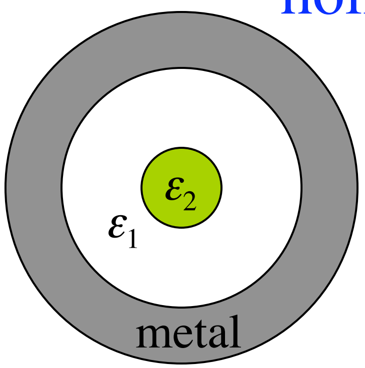
- Possible in left-handed media with $\varepsilon < 0$, $\mu < 0$ for some ω
  — just flip to $\sigma < 0$ in left-handed ω ranges
  [Cummer (2004); Dong *et al*. (2004)]

- Possible in certain waveguides confined by metals or photonic bandgaps…

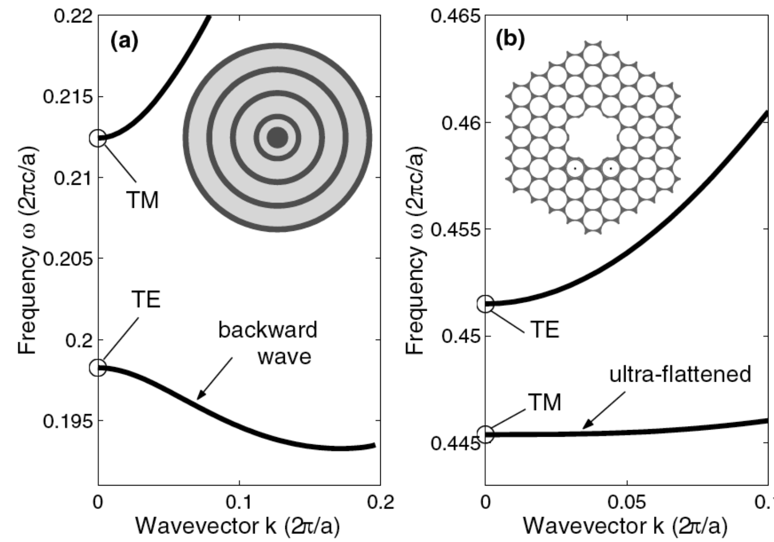
Backward Waveguides

hollow metal tube with inhomogenous core

[Clarricoats & Waldron (1960)]

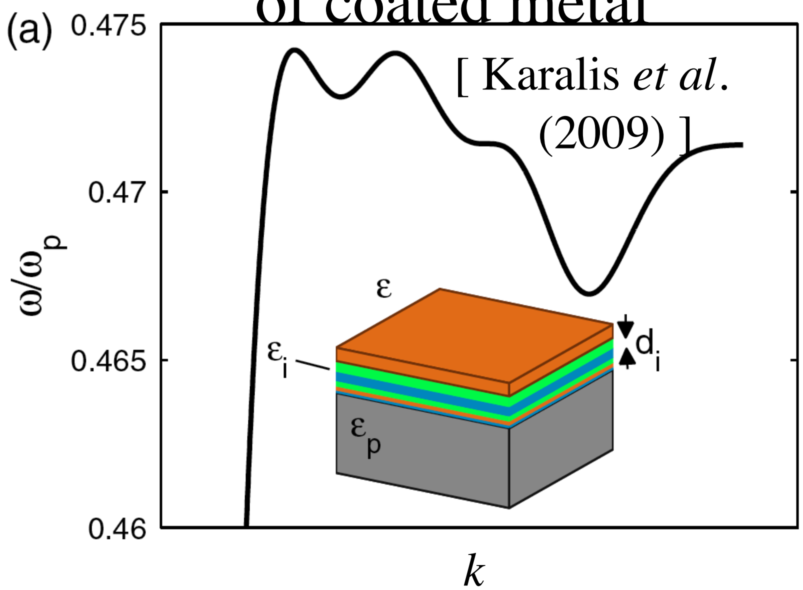


photonic-crystal fibers



[Ibanescu *et al*. (2004)]

surface plasmons of coated metal



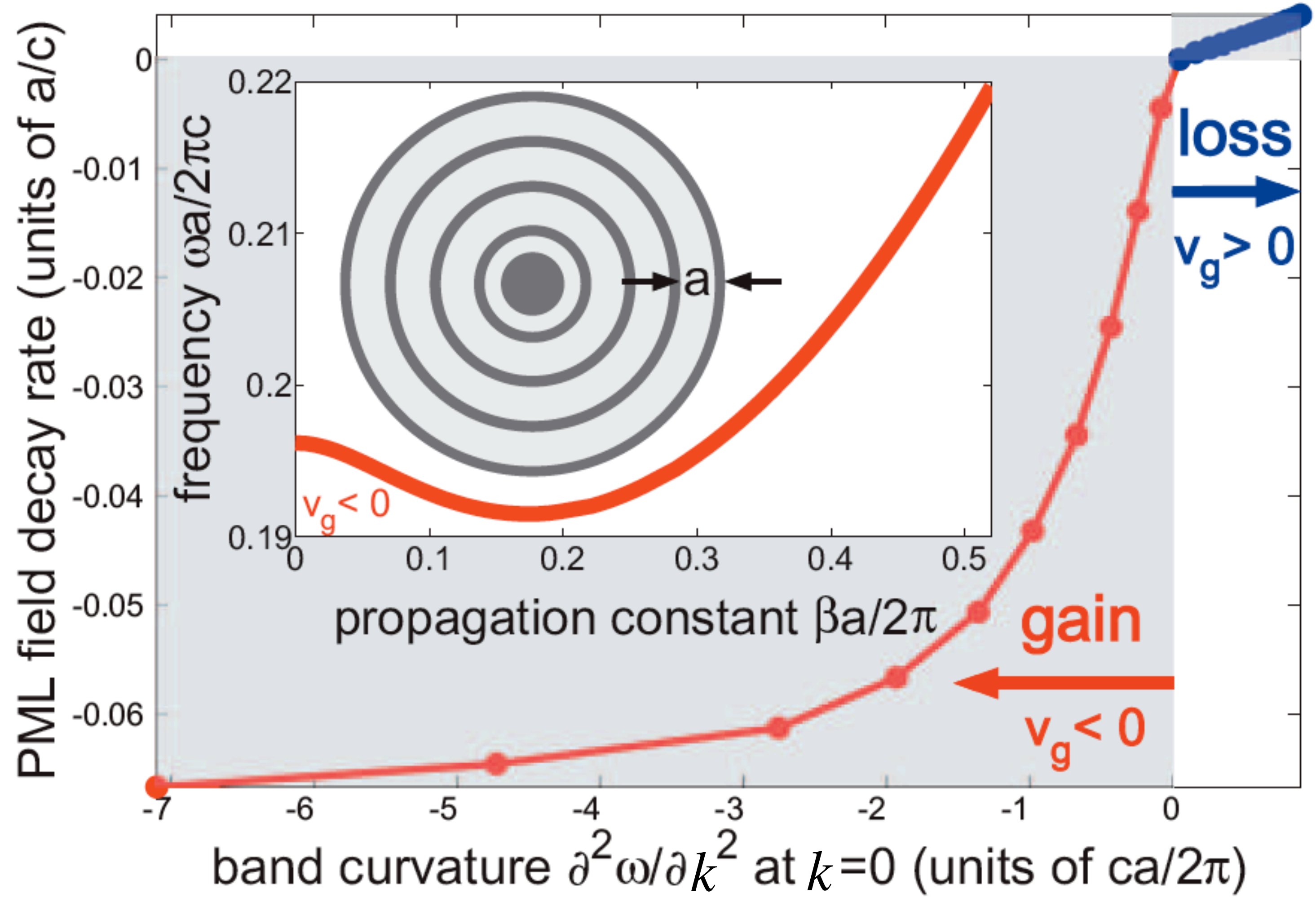
[Karalis *et al*. (2009)]

All have *both* signs of v_g at *same* ω — PML blows up for *any* sign of σ.

[Loh et al, (2009)]

Failure of Backward-Wave PML

[Loh et al, *PRE Rapid Comm*. **79**, 065601 (2009)]



How Can an Absorber Give Gain?

If PML is effectively an anisotropic *absorbing* material, how can *any* field pattern yield exponential growth?

- Answer, part I: it's not exclusively absorbing.

$$\{\varepsilon,\mu\} \to \{\varepsilon,\mu\} \begin{pmatrix} (1+i\sigma/\omega)^{-1} & & \\ & 1+i\sigma/\omega & \\ & & 1+i\sigma/\omega \end{pmatrix}$$

$\mathrm{Im} < 0 \Rightarrow$ gain for *longitudinal* (x) components

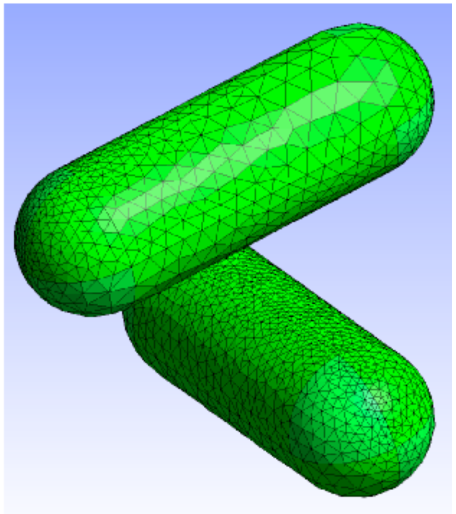
- Answer, part II: backward waves = mostly longitudinal fields

a little-known identity:

$$v_g = v_p \left[\frac{\text{transverse field energy} - \text{longitudinal field energy}}{\text{total field energy}} \right]$$

[Loh *et al.* (2009)]

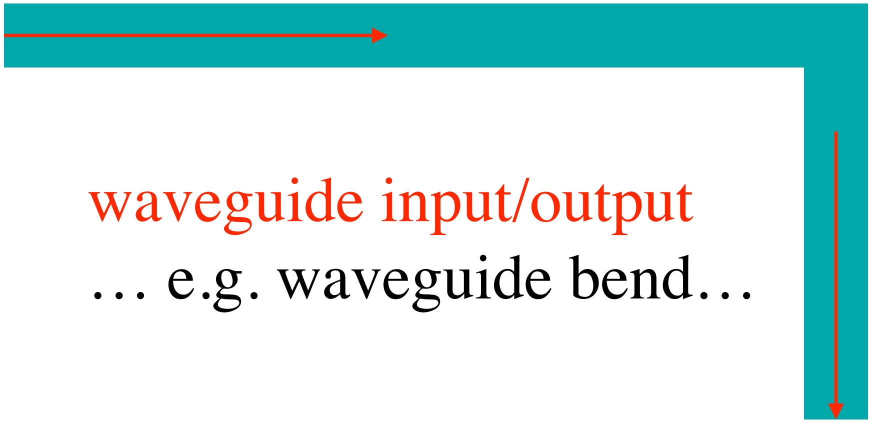
For Those of You Feeling Smug



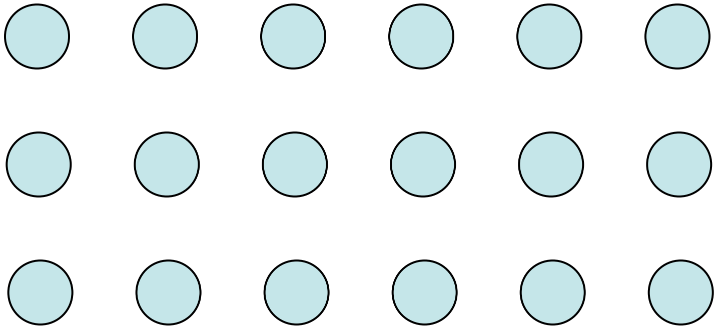
Surface integral-equation methods (e.g. BEM) only discretize *interfaces* and treat ∞ space *analytically*

— *no need for PML!*

… unless one has surfaces extending to ∞ …



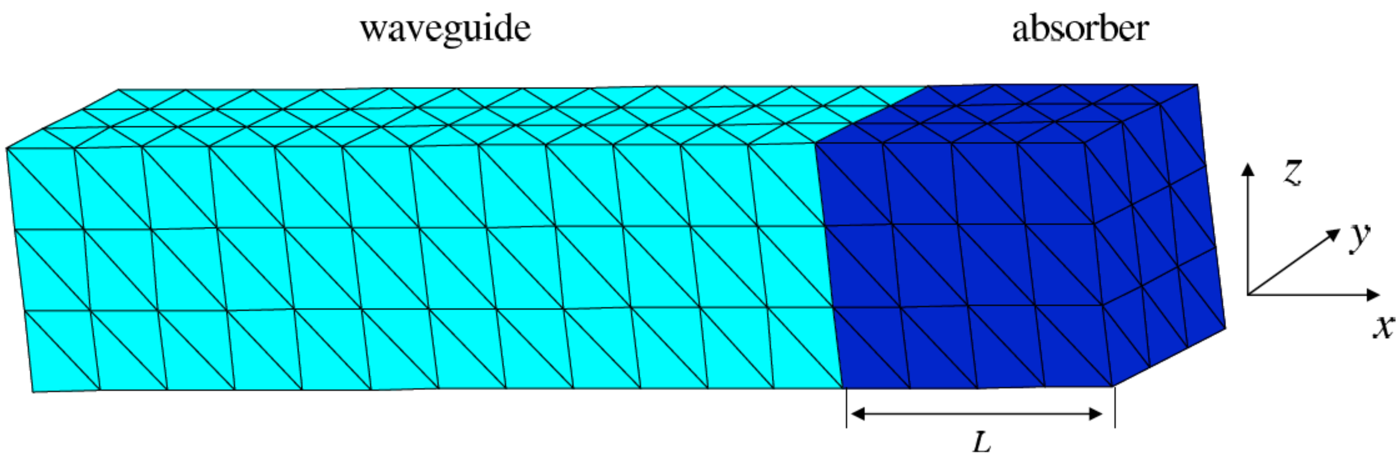
waveguide input/output
… e.g. waveguide bend…



worse, photonic crystals…

Truncating Integral Equations

[Lei Zhang, J. Lee, A. Oskooi, A. Hochman, J. White, S. G. Johnson (2010)]



- want an *adiabatic absorber* truncation — turned on gradually
- must use homogeneous materials for BEM efficiency

⇒ use an *adiabatic* ***surface conductivity***

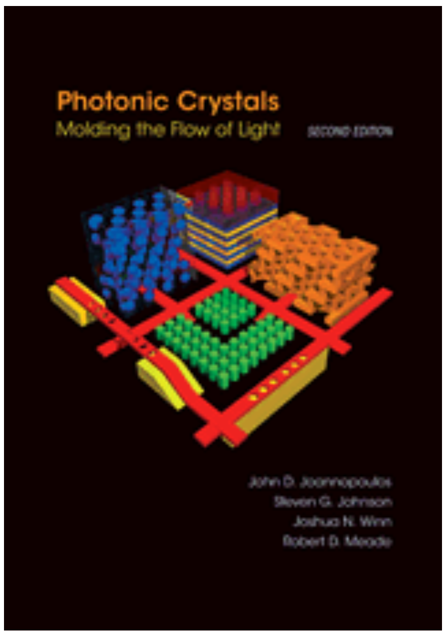
(δ-function σ = jump condition at interface)

~ 10^{-8} reflection with L=10λ

finis

PML is a wonderful tool, but not a panacea.

One fallback is an adiabatic absorber,
but current situation here is still suboptimal.



Photonic Crystals book: http://jdj.mit.edu/book

Papers/preprints: http://math.mit.edu/~stevenj

PML notes: http://math.mit.edu/~stevenj/notes