Optimizing the perfectly matched layer

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Overview

- PML constructed using a change of variables
  - Cartesian coordinates (review)
  - Comparison to Bérenger's approach in cylindrical coordinates
- Discretization of PMLs and resulting effects
- Optimization of cartesian PMLs
- Effects of boundary conditions

Framework: Planar Maxwell equations

PML construction - Overview

We have already seen that a PML can be understood in two ways:

- Split the magnetic field and introduce a damping term σ (Bérenger's approach)
- Perform a complex change of variables

We will see:

1. cartesian case: both are equivalent
2. cylindrical coordinates: inequivalent, efficiency differs

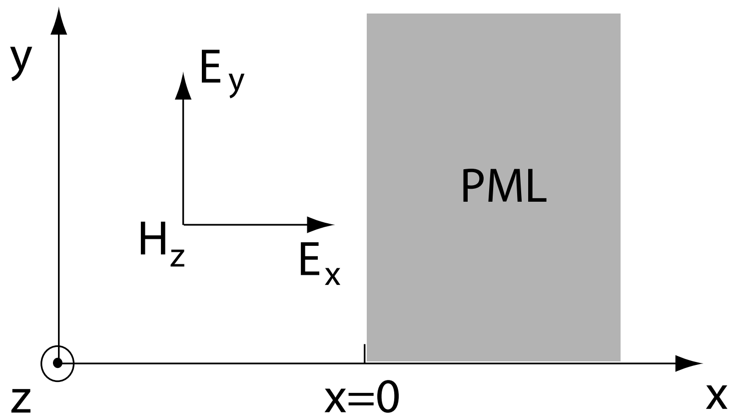
Planar PML for cartesian coords

Consider a TE wave ($E_z = 0$) in free space ($\epsilon_0 = \mu_0 = c = 1$). The two-dimensional Maxwell equations then reduce to:

$$\frac{\partial H_z}{\partial t} = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}$$

$$\frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x} \quad , \quad \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y}$$

Suppose we'd like to construct a 2D PML for $x > 0$:



Bérenger PML for cart. coords

Bérenger:

1. Split H field: $H_z = H_{zx} + H_{zy}$ such that the MW equations can be written as:

$$\frac{\partial H_{zx}}{\partial t} = -\frac{\partial E_y}{\partial x} \quad , \quad \frac{\partial H_{zy}}{\partial t} = \frac{\partial E_x}{\partial y}$$

$$\frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x} \quad , \quad \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y}$$

2. Introduce damping term $\sigma(x)$ ($\sigma(x) = 0$ for $x < 0$) in all equations which contain x-derivatives:

$$\frac{\partial H_{zx}}{\partial t} + \sigma(x) H_{zx} = -\frac{\partial E_y}{\partial x} \quad , \quad \frac{\partial H_{zy}}{\partial t} = \frac{\partial E_x}{\partial y}$$

$$\frac{\partial E_y}{\partial t} + \sigma(x) E_y = -\frac{\partial H_z}{\partial x} \quad , \quad \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y}$$

Bérenger PML for cart. coords II

3. In time harmonic regime,

$$E_i(x,y,t) = \hat{E}_i(x,y)\exp(-i\omega t), \quad H_{zi}(x,y,t) = \hat{H}_{zi}(x,y)\exp(-i\omega t), \; i = x,y \;\; ,$$

the PML equations can be written as:

$$-i\omega\hat{H}_z = \frac{\partial \hat{E}_x}{\partial y} - \frac{1}{1+i\sigma/\omega}\frac{\partial \hat{E}_y}{\partial x},$$

$$-i\omega\hat{E}_y = -\frac{1}{1+i\sigma/\omega}\frac{\partial \hat{H}_z}{\partial x}, \qquad -i\omega\hat{E}_x = \frac{\partial \hat{H}_z}{\partial y}$$

Change of variables technique

1. Start again in time harmonic regime, but don't split fields:

$$E_i(x,y,t) = \hat{E}_i(x,y)\exp(-i\omega t), \quad H_z(x,y,t) = \hat{H}_z(x,y)\exp(-i\omega t), \; i = x,y$$

2. In frequency domain, the Maxwell equations become:

$$\begin{aligned} -i\omega \hat{H}_z &= \frac{\partial \hat{E}_x}{\partial y} - \frac{\partial \hat{E}_y}{\partial x}, \\ -i\omega \hat{E}_y &= -\frac{\partial \hat{H}_z}{\partial x}, \quad -i\omega \hat{E}_x = \frac{\partial \hat{H}_z}{\partial y} \end{aligned}$$

3. Change of variables: $x \to x' = x + \frac{i}{\omega}\int_0^x \sigma(s)ds$

Change of variables technique II

If we use the chain rule to replace x' by x, we get:

$$
\begin{aligned}
-i\omega \hat{H}_z &= \frac{\partial \hat{E}_x}{\partial y} - \frac{1}{1+i\sigma/\omega}\frac{\partial \hat{E}_y}{\partial x}, \\
-i\omega \hat{E}_y &= -\frac{1}{1+i\sigma/\omega}\frac{\partial \hat{H}_z}{\partial x}, \qquad -i\omega \hat{E}_x = \frac{\partial \hat{H}_z}{\partial y}
\end{aligned}
$$

This is exactly the Bérenger PML in the frequency domain: **Both approaches are equivalent!**

Practical computation: truncate PML. We impose Dirichlet BC:

$$\hat{E}_y(x=\delta, y, t) = 0 \qquad \Longrightarrow \qquad R = e^{-2ik_x \int_0^\delta (1+i\sigma(s)/\omega)ds}$$

Note: Pick σ large to minimize R (if $k_x \in \mathbb{R}$).

PML for curvilinear coordinates

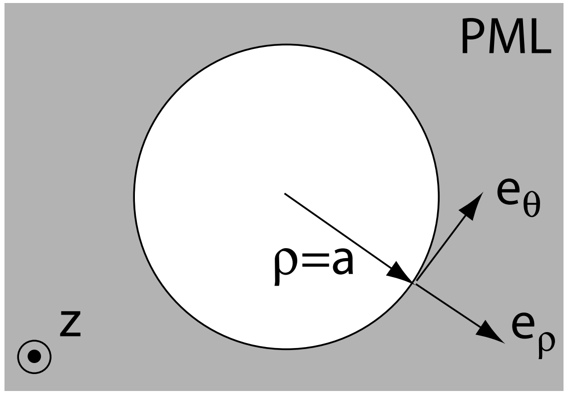
Do Bérenger's and the complex change of variables approach also result in equivalent PMLs for non-Cartesian coordinate system?

Maxwell's equations in polar coordinates (ρ, θ):

$$\frac{\partial H_z}{\partial t} = \frac{1}{\rho}\left(\frac{\partial E_\rho}{\partial \theta} - \frac{\partial}{\partial \rho}(\rho E_\theta)\right)$$

$$\frac{\partial E_\rho}{\partial t} = \frac{1}{\rho}\frac{\partial H_z}{\partial \theta}, \qquad \frac{\partial E_\theta}{\partial t} = -\frac{\partial H_z}{\partial \rho}$$

Assume the layer starts at $\rho = a$, so $\sigma(\rho) > 0$ for $\rho > a$ and 0 otherwise.



Change of variables for polar coords

Start in the frequency domain. Let $\rho' = \rho + \frac{i}{\omega} \int_a^\rho \sigma(s) ds$ and introduce

$$d(\rho) = 1 + i\frac{\sigma(\rho)}{\omega} \quad \text{and} \quad \bar{d}(\rho) = 1 + i\frac{1}{\rho\omega} \int_a^\rho \sigma(s) ds$$

such that $\rho' = \rho\bar{d}$ and $\frac{d\rho'}{d\rho} = d$. We thus have in freq. domain:

$$-i\omega H_z = \frac{1}{\bar{d}\rho}\left(\frac{\partial E_\rho}{\partial\theta} - \frac{1}{d}\frac{\partial}{\partial\rho}(\bar{d}\rho E_\theta)\right)$$

$$-i\omega E_\rho = \frac{1}{\bar{d}\rho}\frac{\partial H_z}{\partial\theta}, \qquad -i\omega E_\theta = -\frac{1}{d}\frac{\partial H_z}{\partial\rho}$$

Note: $\frac{1}{d}\frac{\partial}{\partial\rho} = \frac{\partial}{\partial\rho'} = \frac{\partial}{\partial(\bar{d}\rho)}$

Change of variables for polar coords II

Using $\tilde{E}_\rho = dE_\rho$ and $\tilde{E}_\theta = \bar{d}E_\theta$ we get the traditional Helmholtz equations:

$$-i\omega d\bar{d}H_z = \frac{1}{\rho}\left(\frac{\partial \tilde{E}_\rho}{\partial \theta} - \frac{\partial}{\partial \rho}(\rho \tilde{E}_\theta)\right)$$

$$-i\omega \frac{\bar{d}}{d}\tilde{E}_\rho = \frac{1}{\rho}\frac{\partial H_z}{\partial \theta}, \qquad -i\omega \frac{d}{\bar{d}}\tilde{E}_\theta = -\frac{\partial H_z}{\partial \rho}$$

We can return to time domain by introducing $E^*_\rho = 1/d\tilde{E}_\rho$, $E^*_\theta = 1/\bar{d}\tilde{E}_\theta$, $H^*_z = \bar{d}H_z$ and $\bar{\sigma}(\rho) = \frac{1}{\rho}\int_a^\rho \sigma(s)ds$:

$$\frac{\partial H^*_z}{\partial t} + \sigma H^*_z = \frac{1}{\rho}\left(\frac{\partial \tilde{E}_\rho}{\partial \theta} - \frac{\partial}{\partial \rho}(\rho \tilde{E}_\theta)\right), \qquad \frac{\partial E^*_\rho}{\partial t} + \bar{\sigma}E^*_\rho = \frac{1}{\rho}\frac{\partial H_z}{\partial \theta}, \qquad \frac{\partial E^*_\theta}{\partial t} + \sigma E^*_\theta = -\frac{\partial H_z}{\partial \rho}$$

$$\frac{\partial \tilde{E}_\rho}{\partial t} = \frac{\partial E^*_\rho}{\partial t} + \sigma E^*_\rho, \qquad \frac{\partial \tilde{E}_\theta}{\partial t} = \frac{\partial E^*_\theta}{\partial t} + \bar{\sigma}E^*_\theta, \qquad \frac{\partial H_z}{\partial t} + \bar{\sigma}H_z = \frac{\partial H^*_z}{\partial t}$$

Comparison to Bérenger's PML

In order to compare the two constructions, assume that $\frac{\partial H_z}{\partial \theta} = 0$ and choose $E_\rho = 0$.

$$\Longrightarrow \frac{\partial H_z^*}{\partial t} + \sigma H_z^* = -\frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho \tilde{E}_\theta), \qquad \frac{\partial E_\theta^*}{\partial t} + \sigma E_\theta^* = -\frac{\partial H_z}{\partial \rho}$$

$$\frac{\partial \tilde{E}_\theta}{\partial t} = \frac{\partial E_\theta^*}{\partial t} + \bar{\sigma} E_\theta^*, \qquad \frac{\partial H_z}{\partial t} + \bar{\sigma} H_z = \frac{\partial H_z^*}{\partial t}$$

Bérenger's construction would yield:

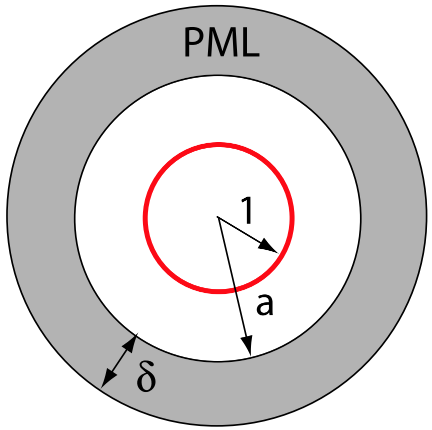
$$\frac{\partial H_z}{\partial t} + \sigma H_z = -\frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho E_\theta), \qquad \frac{\partial E_\theta}{\partial t} + \sigma E_\theta = -\frac{\partial H_z}{\partial \rho}$$

They are clearly different!

Question: How do they perform qualitatively?

Comparison to Bérenger’s PML II

Think of the following setup:



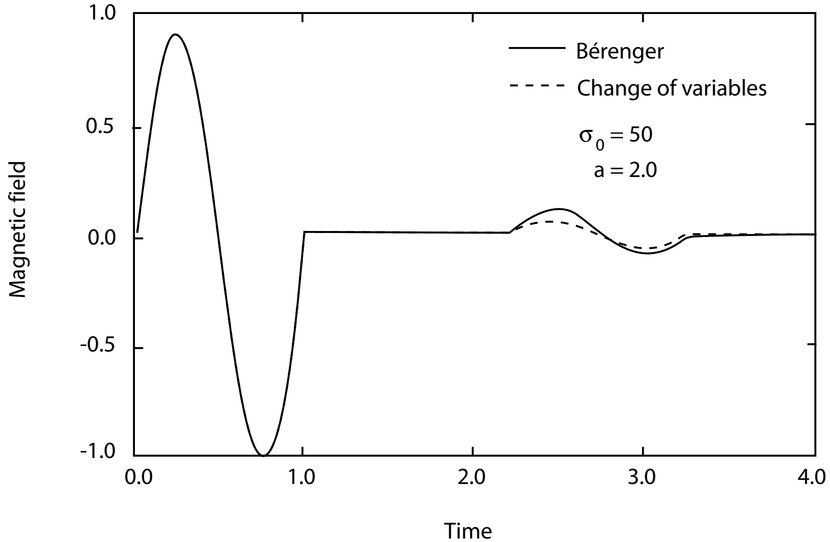
We take the source to be on the unit disc,

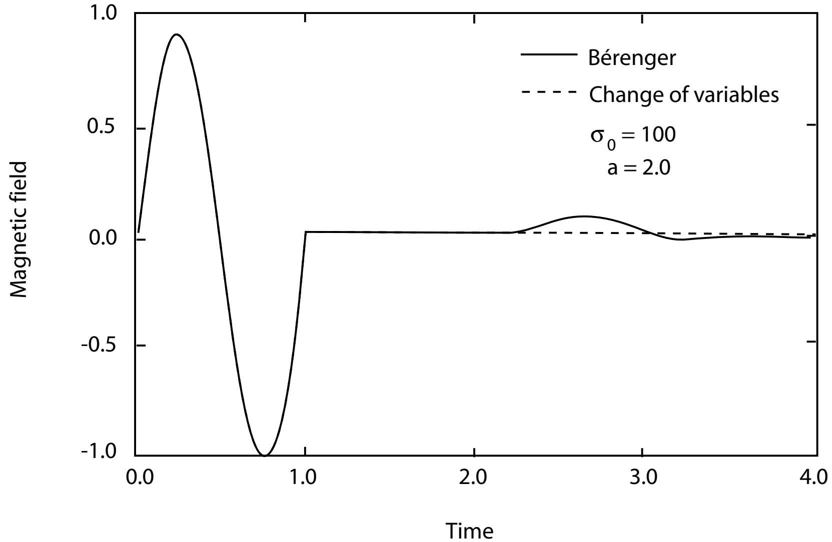
At $\rho = 1$: $\quad E_\theta = \sin(2\pi t)$ for $0 \leq t \leq 1$ and 0 otherwise,

and choose a quadratic ρ-dependance for σ:

$$\sigma(\rho) = \sigma_0(\rho - a)^2/\delta^2, \text{ for } \rho \geq a$$

Comparison to Bérenger's PML III



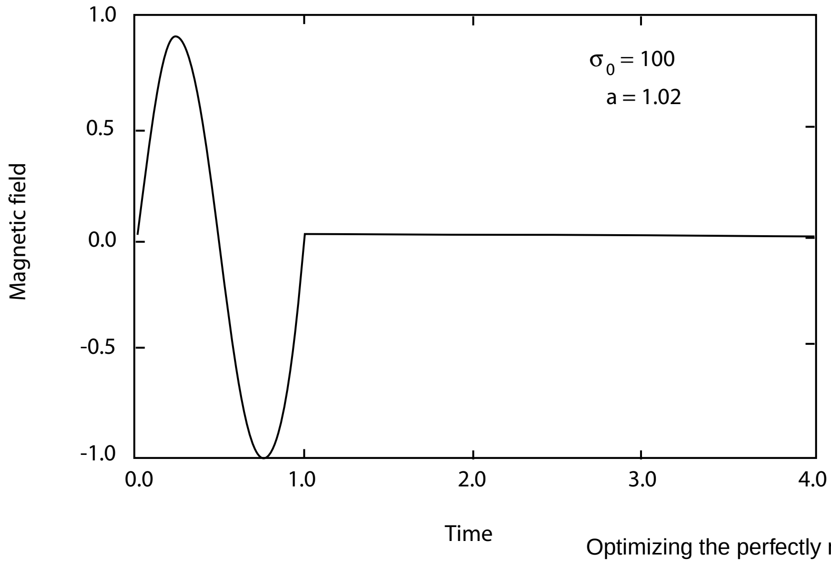


Parameters:

N = 100 (number of points)
$n_l = 10$ (number of points in PML)
h = (a-1)/N (spacing)
$\delta = n_l h$ (layer thickness)

$\sigma(\rho) = \sigma_0 (\rho - a)^2 / \delta^2$

All plots show H_z at x = h/2 (ie. close to the scatterer)



Conclusions

- The change of variables PML gives a much more accurate (discrete) absorbing layer than Bérenger's construction in polar coordinates.
- Unlike Bérenger's PML, the change of variables technique allows tuning of PMLs situated very close to the scatterer, yet producing very good absorption.
- The quality of our PML still depends on a number of parameters (including discretization params) which need to be chosen wisely.

$\Longrightarrow$ Is there a way to quantify the effects of discretization? Furtermore, can we derive optimal PML parameters from there?

Effects of discretization

For simplicity, we restrict ourselves to the planar, two-dimensional case. Starting from Bérenger's construction, we avoid the split fields by defining:

$$\tilde{E}_x = (1 + i\sigma/\omega)\hat{E}_x, \qquad \tilde{E}_y = \hat{E}_y, \qquad \tilde{H}_z = \hat{H}_z$$

Now we have again a traditional curl-curl structure:

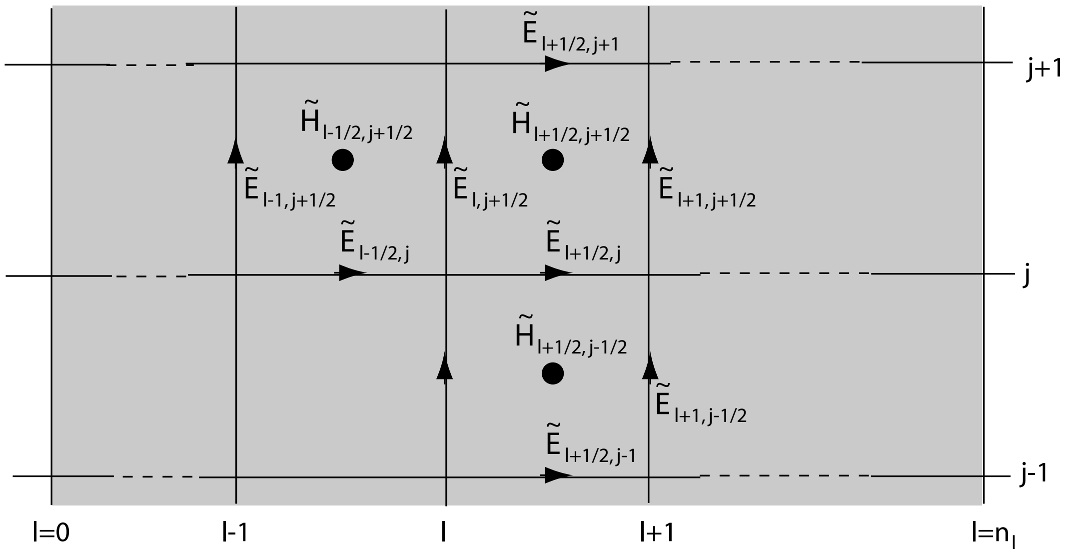
$$-i\omega(1 - i\sigma/\omega)\tilde{H}_z = \frac{\partial \tilde{E}_x}{\partial y} - \frac{\partial \tilde{E}_y}{\partial x}$$

$$-i\omega(1 - i\sigma/\omega)\tilde{E}_y = -\frac{\partial \tilde{H}_z}{\partial x}, \qquad -\frac{i\omega}{1 + i\sigma/\omega}\tilde{E}_x = \frac{\partial \tilde{H}_z}{\partial y}$$

Discretization of planar PML

We use
a standard Yee scheme and let $\sigma(x)$ be
piecewise constant with jumps at $x = lh$,
$l = 0, 1, 2, \ldots$. We denote by $\sigma_{l+1/2}$
the value of σ in the interval $(lh, (l+1)h)$.

We then arrive
at the following discretized equations:



$$-i\frac{\omega}{\gamma_{l+1/2}}\tilde{E}_{l+1/2,j} = \frac{\tilde{H}_{l+1/2,j+1/2} - \tilde{H}_{l+1/2,j-1/2}}{h}$$

$$-i\omega\frac{\gamma_{l+1/2} + \gamma_{l-1/2}}{2}\tilde{E}_{l,j+1/2} = -\frac{\tilde{H}_{l+1/2,j+1/2} - \tilde{H}_{l-1/2,j+1/2}}{h}$$

$$-i\omega\gamma_{l+1/2}\tilde{H}_{l+1/2,j+1/2} = \frac{\tilde{E}_{l+1/2,j+1} - \tilde{E}_{l+1/2,j}}{h} - \frac{\tilde{E}_{l+1,j+1/2} - \tilde{E}_{l,j+1/2}}{h}$$

with $\gamma_{l+1/2} = 1 + i\sigma_{l+1/2}/\omega$.

Discretization of planar PML II

To make life easier: Assume $\tilde{H}_{l+1/2,j+1/2} = e^{i\kappa_2(j+1/2)h}\tilde{H}_{l+1/2}$ and eliminate the various $\tilde{E}$'s to get an expression for $\tilde{H}$ only:

$$
\begin{aligned}
-h^2\omega^2\lambda\gamma_{l+1/2}\tilde{H}_{l+1/2} &= \frac{2}{\gamma_{l+3/2}+\gamma_{l+1/2}}(\tilde{H}_{l+3/2}-\tilde{H}_{l+1/2}) \\
&\quad -\frac{2}{\gamma_{l+1/2}+\gamma_{l-1/2}}(\tilde{H}_{l+1/2}-\tilde{H}_{l-1/2})
\end{aligned}
$$

where we defi ned $\lambda = 1 - \frac{4}{h^2\omega^2}\sin^2(\kappa_2 h/2)$.

To fi nd the reflection coeffi cientdue to the discretization, we'll use $\sigma = const$, thus $\gamma = \gamma_{l+1/2} = const$ and use the plain wave ansatz

$$
\begin{aligned}
\tilde{H}_{l+1/2} &= e^{i\kappa_1 h(l+1/2)} + Re^{-i\kappa_1 h(l+1/2)} && \text{for } l \leq -1 \quad (x<0) \\
\tilde{H}_{l+1/2} &= Te^{i\kappa_1^\sigma h(l+1/2)} && \text{for } l \geq 0 \text{ (inside PML)}
\end{aligned}
$$

Discretization of planar PML III

Using this ansatz to solve the discrete $\tilde{H}$ equations at the interface (corresponding to $x = 0$), we can derive an expression for the reflection coeffcient R for an *infinite* layer:

$$R = \frac{1}{16}(\omega^2 - \kappa_2^2)\frac{\sigma(\sigma - 2\omega i)}{\omega^2}h^2 + O(h^4)$$

Discretizing the PML has introduced a reflection from the interface at $x = 0$.

The layer is thus no longer perfectly matched . **As R is of magnitude $\sigma^2 h^2$, we cannot choose σ arbitrarily large anymore.**

Before dealing with an optimal choice of σ, we will consider the case of a *finite* layer.

Refl. coeff. for finite, discrete PMLs

Suppose a PML thickness of $\delta = n_l \cdot h$. The discretized equations at $l = n_l - 1$ will require the value of the boundary data. If we choose Dirichlet BC, we can set $\tilde{E}_{n_l,j+1/2} = 0, \quad \forall j$. Remember:

$$
\begin{aligned}
-i\omega\gamma\tilde{E}_{n_l,j+1/2} &= -\frac{\tilde{H}_{n_l+1/2,j+1/2} - \tilde{H}_{n_l-1/2,j+1/2}}{h}, \\
-h^2\omega^2\lambda\gamma\tilde{H}_{l+1/2} &= \frac{1}{\gamma}(\tilde{H}_{l+3/2} - \tilde{H}_{l+1/2}) - \frac{1}{\gamma}(\tilde{H}_{l+1/2} - \tilde{H}_{l-1/2})
\end{aligned}
$$

Given $\tilde{H}_{-3/2}$, we can therefore compute

$$\vec{H} = (\tilde{H}_{-1/2}, \tilde{H}_{1/2}, \ldots, \tilde{H}_{n_l-1/2})^\top$$

Refl. coeff. for fi nite, discrete PMLs II

It is easier to calculate $\vec{H}$ in terms of the matrix equation

$$M\vec{H} = -\tilde{H}_{-3/2}\vec{F}$$

where $\vec{F} = (1, 0, \cdots, 0)^\top$ and $M = \begin{pmatrix} c_{-1/2} & d_{1/2} & 0 & \cdots & & \\ d_{1/2} & c_{1/2} & d_{3/2} & 0 & \cdots & \\ 0 & d_{3/2} & c_{3/2} & d_{5/2} & \cdots & \\ & & \ddots & \ddots & \ddots & \\ & \cdots & 0 & d_{n_l-3/2} & c_{n_l-1/2} & \end{pmatrix}$

with

$$\begin{aligned} c_{j+1/2} &= h^2\omega^2\lambda\gamma_{j+1/2} - \frac{2}{\gamma_{j+3/2}+\gamma_{j+1/2}} - \frac{2}{\gamma_{j+1/2}+\gamma_{j-1/2}}, \quad -1 \le j \le n_l - 2 \\ d_{j+1/2} &= 2/(\gamma_{j+1/2}+\gamma_{j-1/2}), \quad 0 \le j \le n_l - 1, \\ c_{n_l-1/2} &= h^2\omega^2\lambda\gamma_{n_l-1/2} - 2/(\gamma_{n_l-1/2}+\gamma_{n_l-3/2}) \end{aligned}$$

Refl. coeff. for fi nite, discrete PMLs III

An expression for the reflection coefficient is then given by

$$R_{dis} = -\frac{1 + F^\top \cdot M^{-1} \cdot F \cdot e^{-i\kappa_1 h}}{1 + F^\top \cdot M^{-1} \cdot F \cdot e^{i\kappa_1 h}}$$

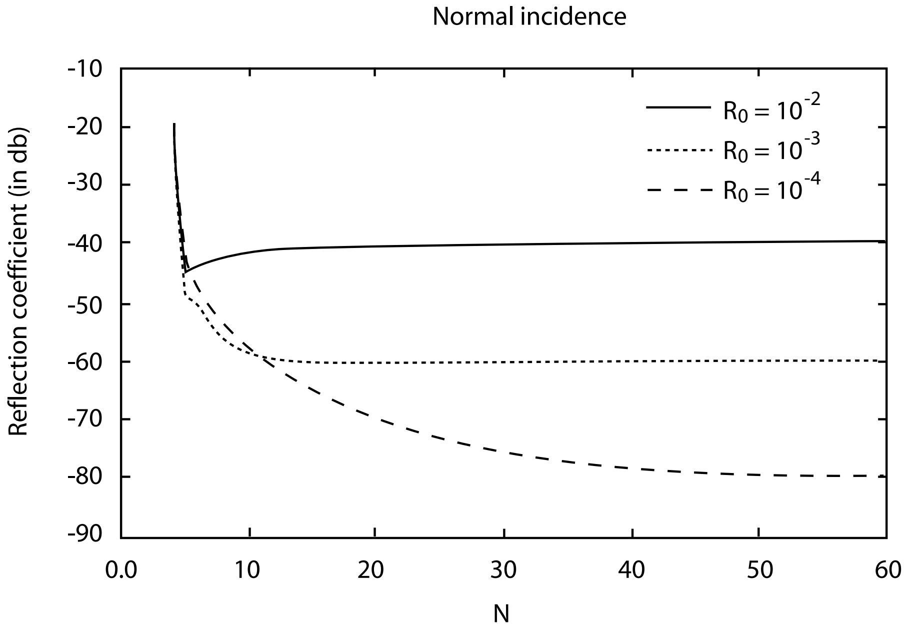
Numerical results: We choose

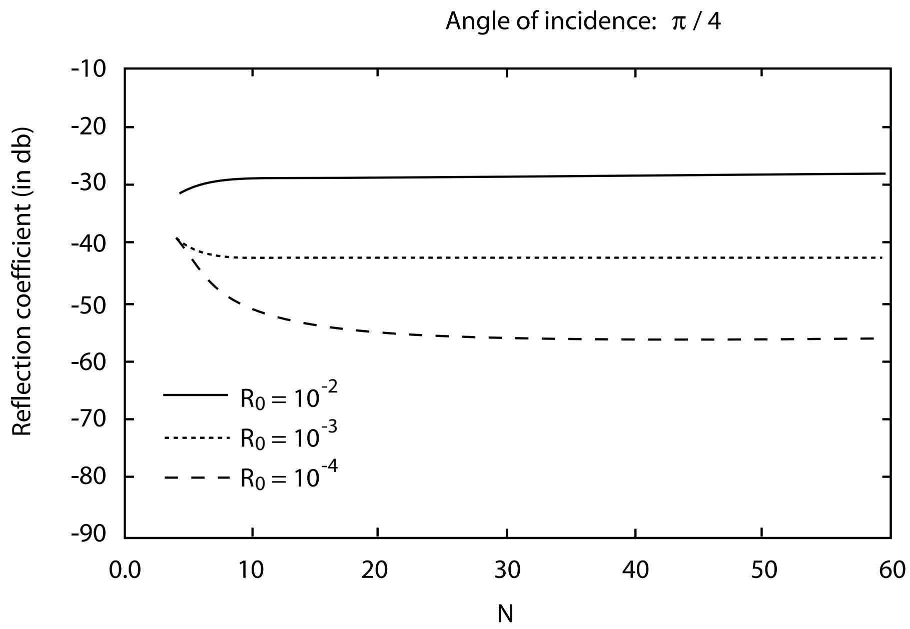
$$\begin{aligned}
\delta = n_l h &= 2\pi/\omega && \text{(layer thickness } = 1 \text{ wavelength)} \\
\sigma(x) &= \sigma_0 (x/\delta)^2, \text{ for } x > 0 && \text{(parabolic law)} \\
\sigma_0 &= \frac{3}{2\delta} \log(\frac{1}{R_0}) \\
N &= 2\pi/(\omega h) && \text{(number of points per wavelength)}
\end{aligned}$$

The choice of σ_0 ensures that the reflection coefficient for the *continuous* model at *normal incidence* is just given by R_0

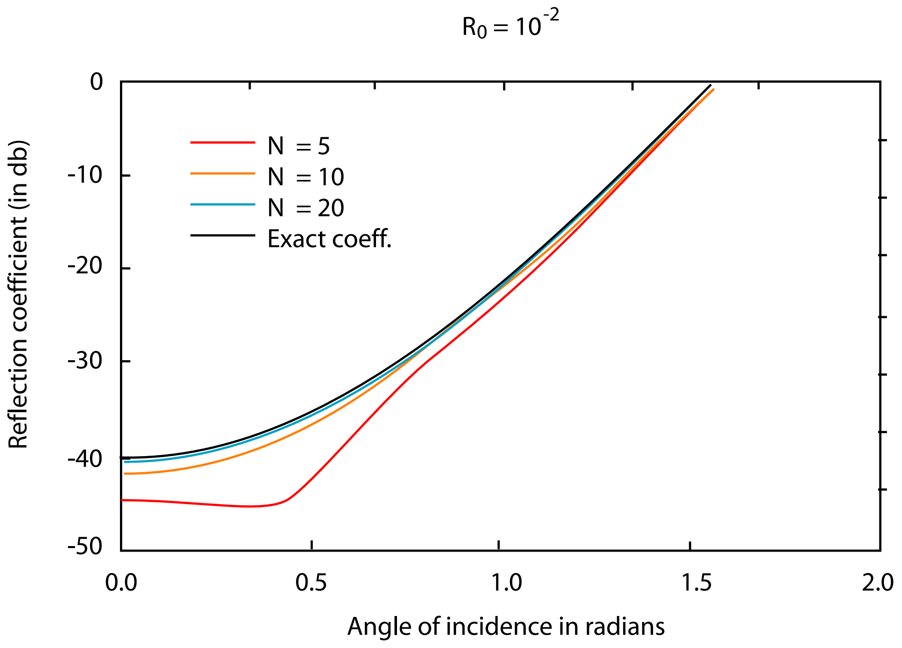
(Remember: $R_{cont} = e^{-2ik_x \int_0^\delta (1+i\sigma(s)/\omega) ds}$ for continuous models).

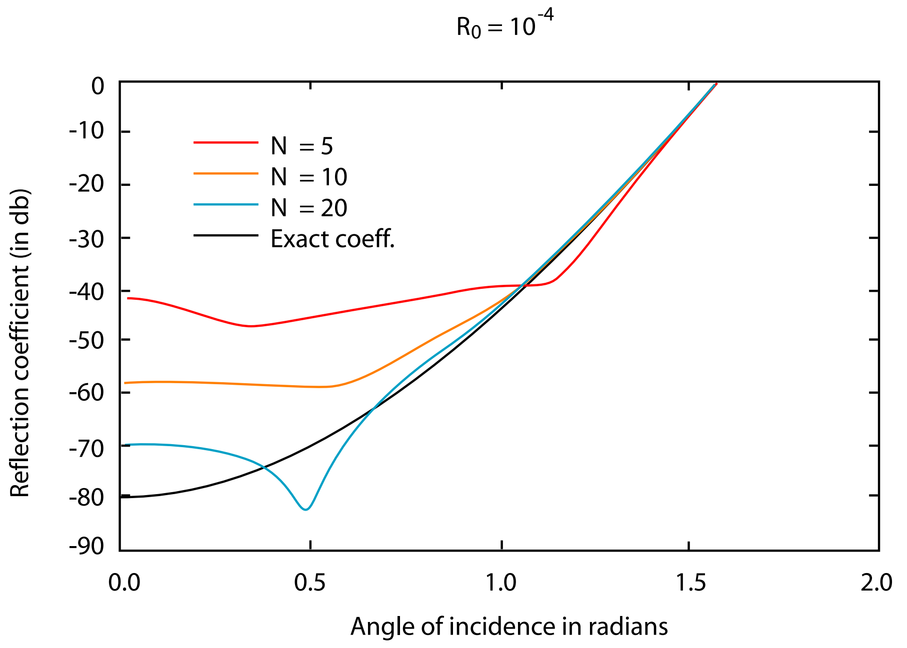
Numerical results I





Numerical results II





Conclusions

- The numerical reflection coefficient converges to the derived value for the continuous model when N is increased.
- The convergence appears to be slower for smaller R_0 (ie. for larger σ_0).
- For fixed N, the largest value of σ_0 does not necessarily result in the smallest reflection coefficient.

Question: Can we choose σ in a better way in order to optimize the effects introduced by discretization?

Optimization of the cart. PML

For practical reasons: For a given N (number of points per wavelength) and n_l (number of points in the layer), what is the best σ to use?

$\Longrightarrow$ Introduce (discrete) $\vec{\sigma}$:

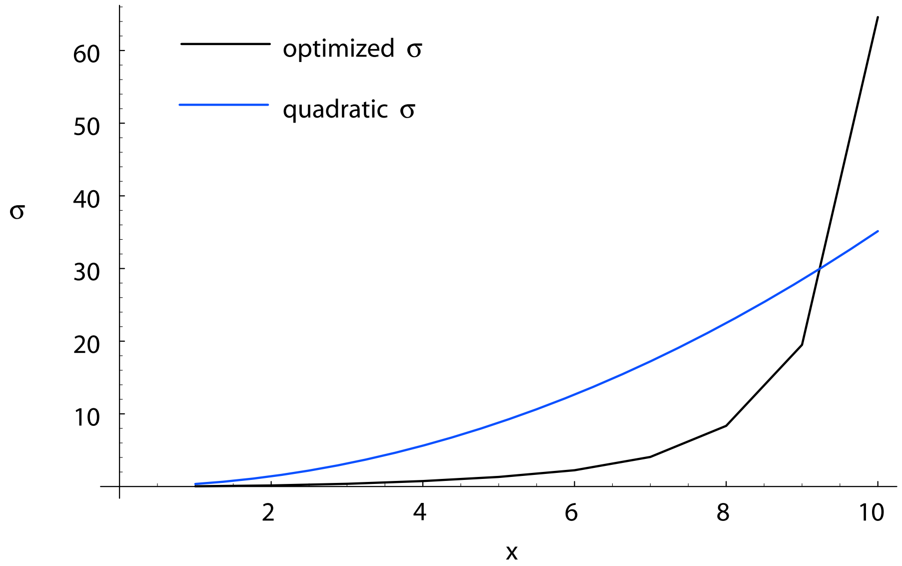
$$\vec{\sigma} = (h\sigma_{1/2}, h\sigma_{3/2}, \ldots, h\sigma_{n_l-1/2})$$

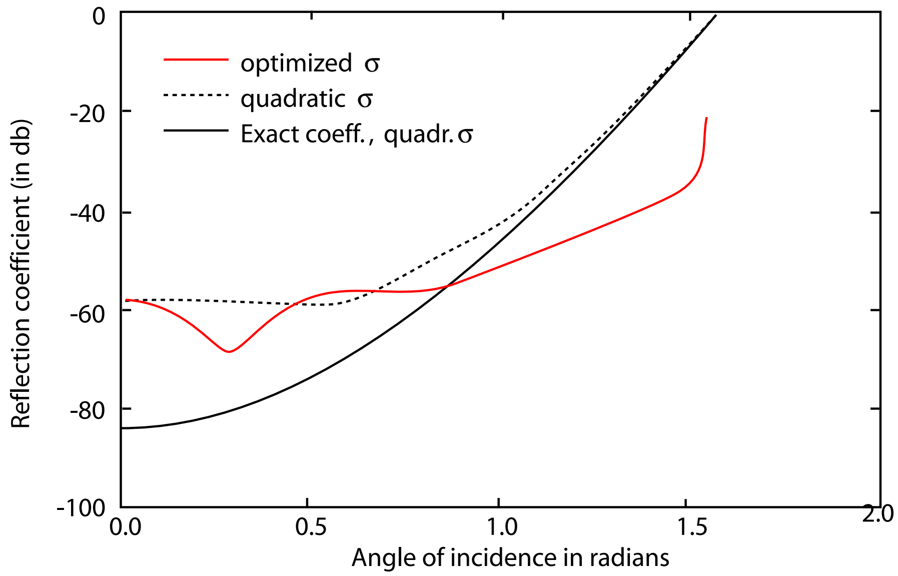
$\vec{\sigma}$ is then found by minimizing R for all angles of incidence. We can - as an example - emphasize *normal* incidence by a $\cos\theta$ weight, thus minimize

$$\frac{1}{100}\sum_{q=1}^{100}\cos(\theta_q)|R(\theta, N, \vec{\sigma})|^2,$$

where $\theta_q = \pi(q-1)/200$.

Numerical results





- Optimal σ profi le is not quadraticanymore.
- The optimized σ improves the *average* reflection coeffi cient.
- The improvement is best for non-normal incidence.

Effects of boundary conditions

We have already seen: Dirichlet BCs lead to additional reflections.

Idea: Use absorbing boundary conditions (ABC) at the end of the PML layer:

$$\tilde{E}_y = \tilde{H}_z \quad \text{on } x = \delta \qquad \text{(Silver-Müller radiation cond.)}$$

$\Rightarrow$ It will clearly influence $\tilde{H}_{n_l - 1/2}$.

Start with the Maxwell equation at the layer end $x = \delta = n_l h$:

$$(-i\omega + \sigma(x))\tilde{E}_y = -\frac{\partial \tilde{H}_z}{\partial x}$$

Using a special FD scheme, it can be discretized in the following form

$$-i\omega\gamma_{n_l - 1/2}\tilde{E}_{n_l, j+1/2} = -\frac{\tilde{H}_{n_l, j+1/2} - \tilde{H}_{n_l - 1/2, j+1/2}}{h/2}.$$

Effects of boundary conditions II

But, as imposed by our boundary conditions, $\tilde{H}_{n_l,j+1/2} = \tilde{E}_{n_l,j+1/2}$, this simplifi es to:

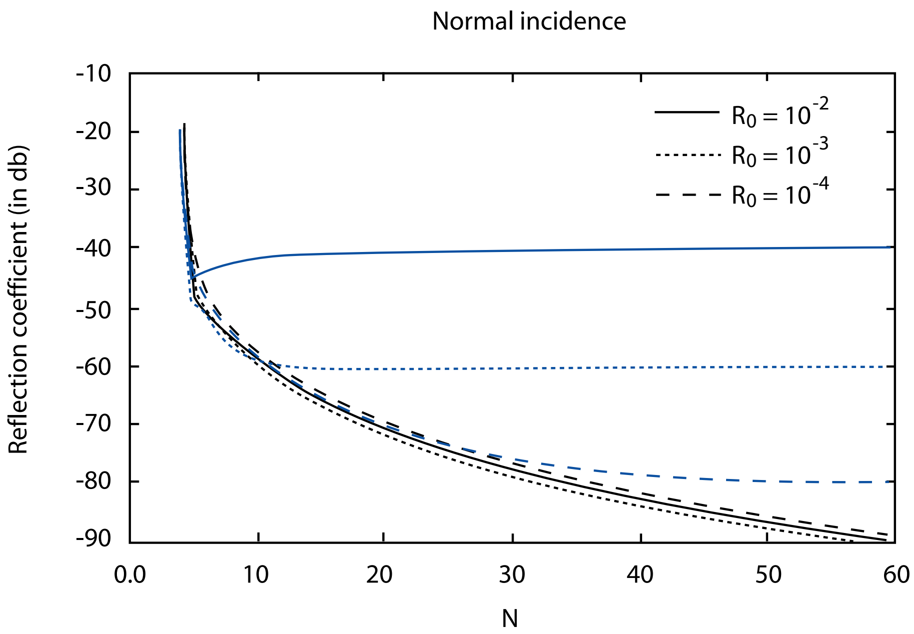
$$-i\omega h\left(\frac{\gamma_{n_l-1/2}}{2} + \frac{i}{\omega h}\right)\tilde{E}_{n_l,j+1/2} = \tilde{H}_{n_l-1/2,j+1/2}$$

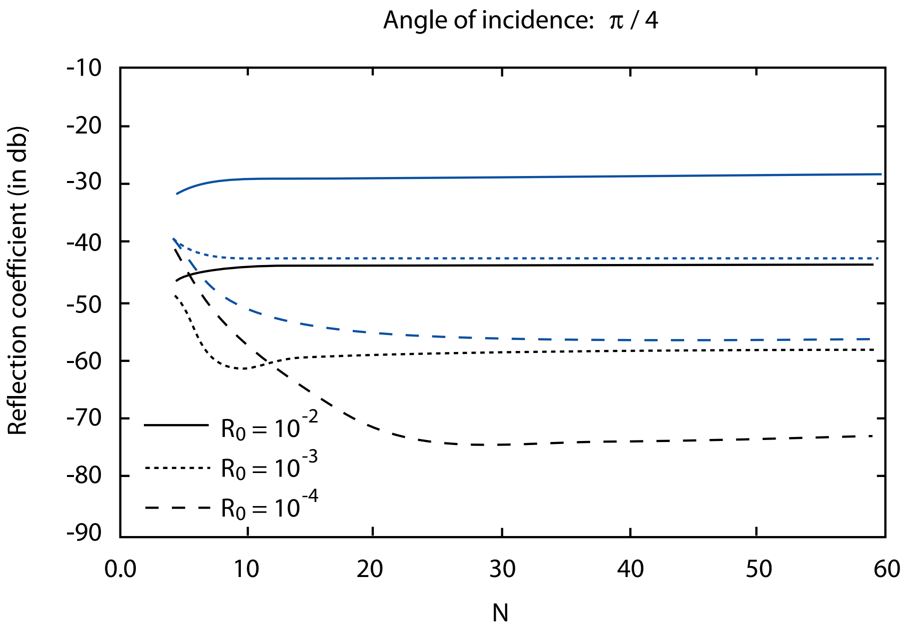
We can now proceed as with Dirichlet BCs: Split away the j part and defi ne $\vec{H} = (\tilde{H}_{-1/2}, \cdots, \tilde{H}_{n_l-1/2})$ and M such that $M\vec{H} = -\tilde{H}_{-3/2}\vec{F}$.

Due to our new boundary conditions, only the last line in M will change, corresponding to the different expression for $\tilde{H}_{n_l-1/2}$. The reflection coeffi cient, however, is still given by the same formula derived earlier:

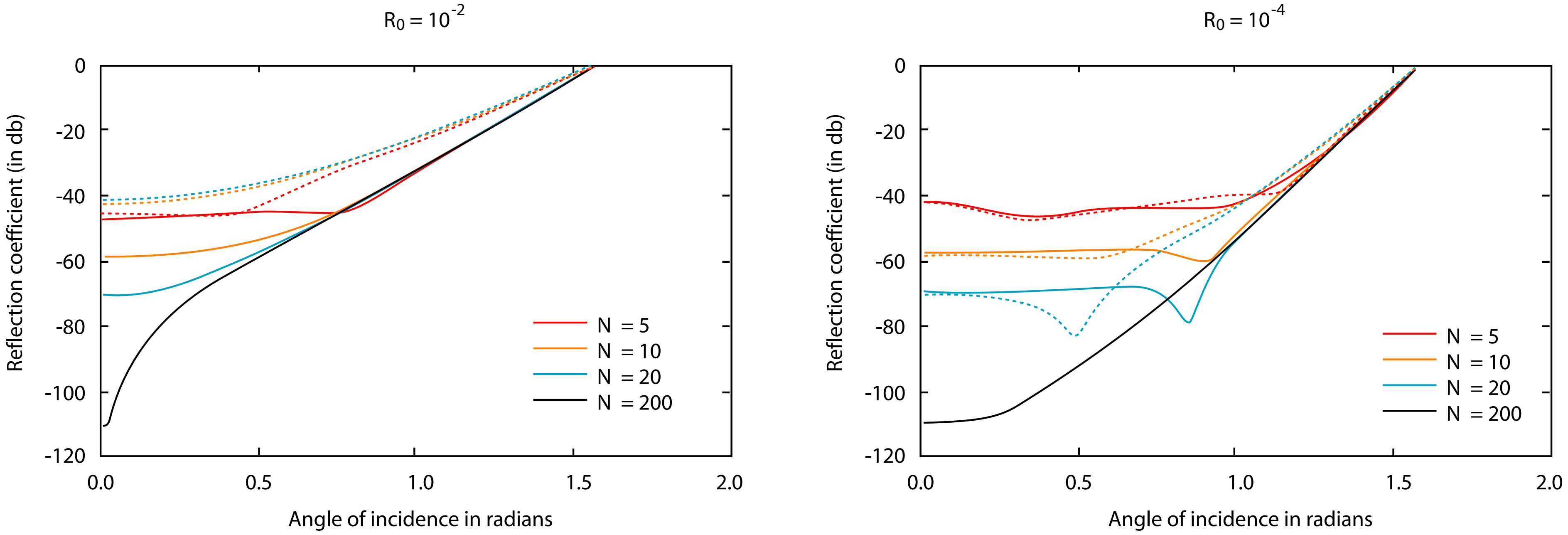
$$R = -\frac{1 + F^\top \cdot M^{-1} \cdot F \cdot e^{-i\kappa_1 h}}{1 + F^\top \cdot M^{-1} \cdot F \cdot e^{i\kappa_1 h}}$$

Numerical results





Numerical results II



Conclusions

- Using ABC's the reflection coefficient converges to zero with higher accuracy. This is what we expect, since our ABC's are perfect, at least for normal wave incidence.
- For parabolic σ, the ABC's improve the reflection for waves close to normal incidence.
- Not shown: Optimizing σ for ABC's does not result in a large improvement, compared to the parabolic case.

Summarized: Absorbing boundary conditions can be considered an enhancement for parabolic σ, especially for normal incidence.

To come to an end...

We have seen that

- PMLs can be generalized to curvilinear coordinates using a complex change of variables, which is superior to Bérenger's construction.
- the effects of discretization can be quantified and we have derived an expression for the reflection coefficient for both, the infinite and the finite layer.
- in order to improve the (discrete, finite) layer, we can optimize σ. However, the parabolic profile is almost optimal.
- using ABC's is worth while for parabolic σ profiles. An optimized profile, however, will then not lead to great improvement.

Questions?