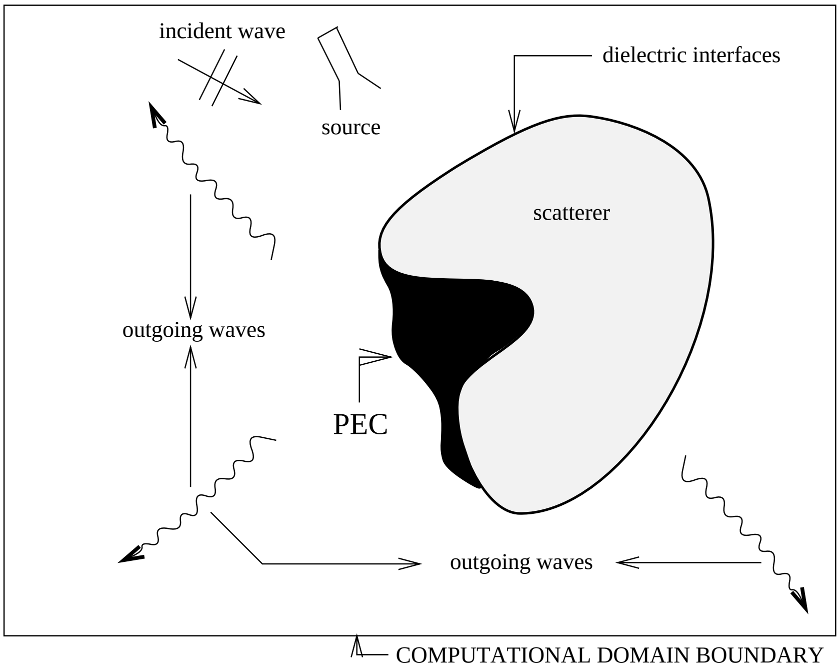
–Fundamentals of a 2nd-order scheme for CEM

We will work with the equations for the Transverse Magnetic (TM) polarization in a non-magnetic dielectric:

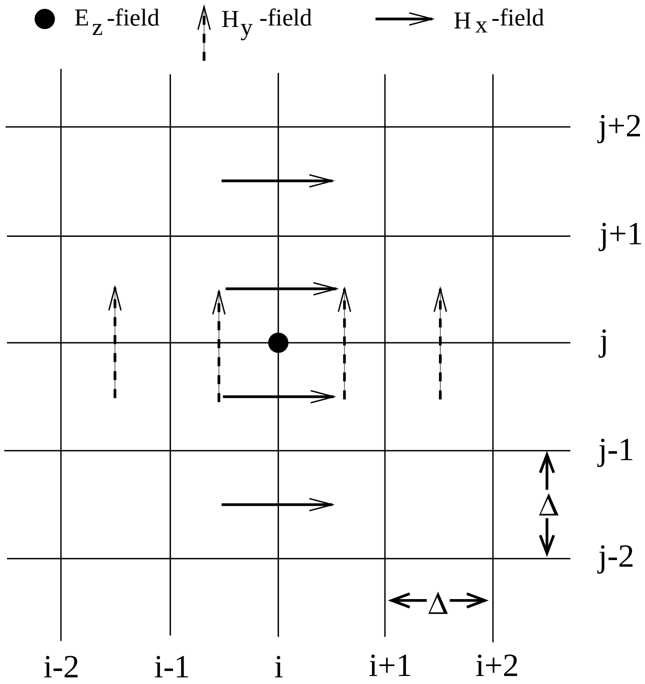
$$
\begin{aligned}
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right), \\
\frac{\partial H_x}{\partial t} &= -\frac{1}{\mu_0}\frac{\partial E_z}{\partial y}, \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu_0}\frac{\partial E_z}{\partial x}
\end{aligned}
$$

In this case, Gauss' Law is trivially satisfied by $\mathbf{D} = (0, 0, \epsilon E_z)^T$, and $\nabla \cdot (H_x, H_y, 0)^T = 0$ for all time.

- Typical computational domain



- The discrete space



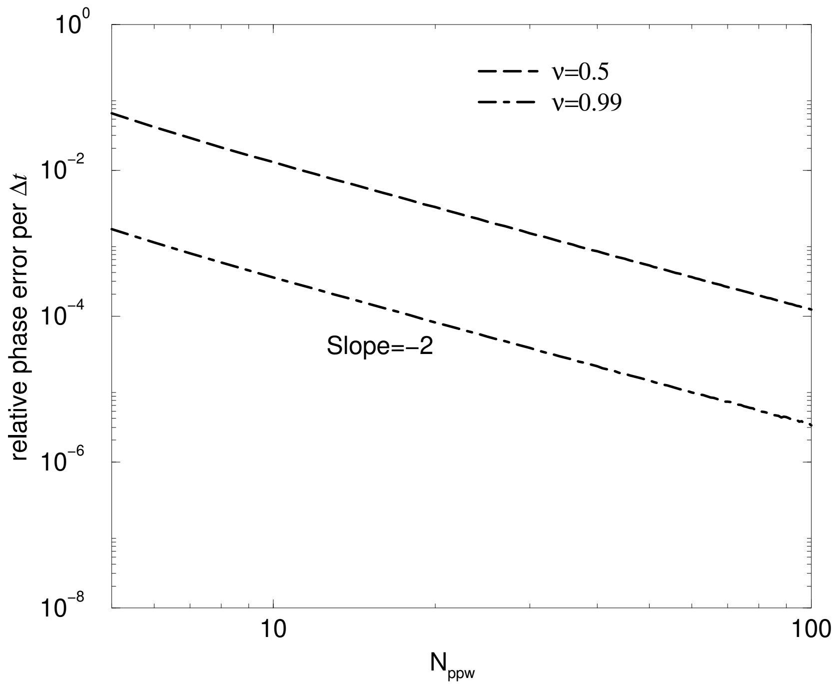
$$
\begin{aligned}
\mu_0 T(HX^n)_{i+\frac{1}{2},j} &= -L^y(EZ^n)_{(i+\frac{1}{2},j)} \\
\mu_0 T(HY^n)_{i,j+\frac{1}{2}} &= L^x(EZ^n)_{(i,j+\frac{1}{2})} \\
\epsilon_{i,j} T(EZ^{n+\frac{1}{2}})_{i,j} &= L^x(HY^{n+\frac{1}{2}})_{(i,j)} - L^y(HX^{n+\frac{1}{2}})_{(i,j)}
\end{aligned}
$$

where $\epsilon_{i,j}$ is the pointwise permittivity except on a dielectric interface, and the difference operators are

$$L^{x(y)} = \frac{S^{1/2} - S^{-1/2}}{\Delta},\ T = \frac{S^{1/2} - S^{-1/2}}{\Delta t}$$

with $S^{\pm\frac{1}{2}}$ being the forward/backward half-cell shift operator. The necessary and sufficient stability condition is $\nu = \frac{c_{max}\Delta t}{\Delta} \leq \frac{1}{\sqrt{d}}$, where $d = 1, 2, 3$ is the # of spatial dimensions ($d = 2$ above) and $c_{max} = max\{1/\sqrt{\epsilon_{i,j}\mu_0}\}$ is the wavefront speed. We call ν the CFL number.

• Dispersion error for propagation along $\theta =$ ...45^o and $\nu = 0.5$

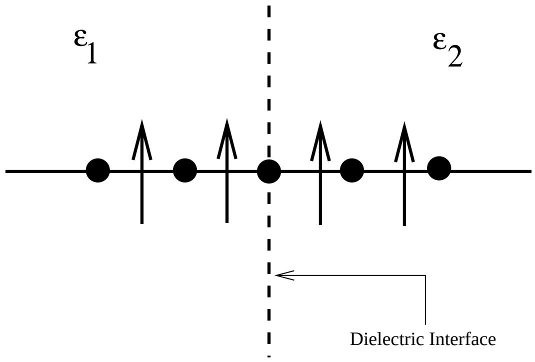


For small $\frac{\pi}{N_{ppw}}$ we have

$$N_{ppw} \approx (\tfrac{1}{3})^{\frac{1}{2}} \pi^{\frac{3}{2}} (sin^4\theta + cos^4\theta)^{\frac{1}{2}} (\tfrac{J}{e_\phi})^{\frac{1}{2}},$$

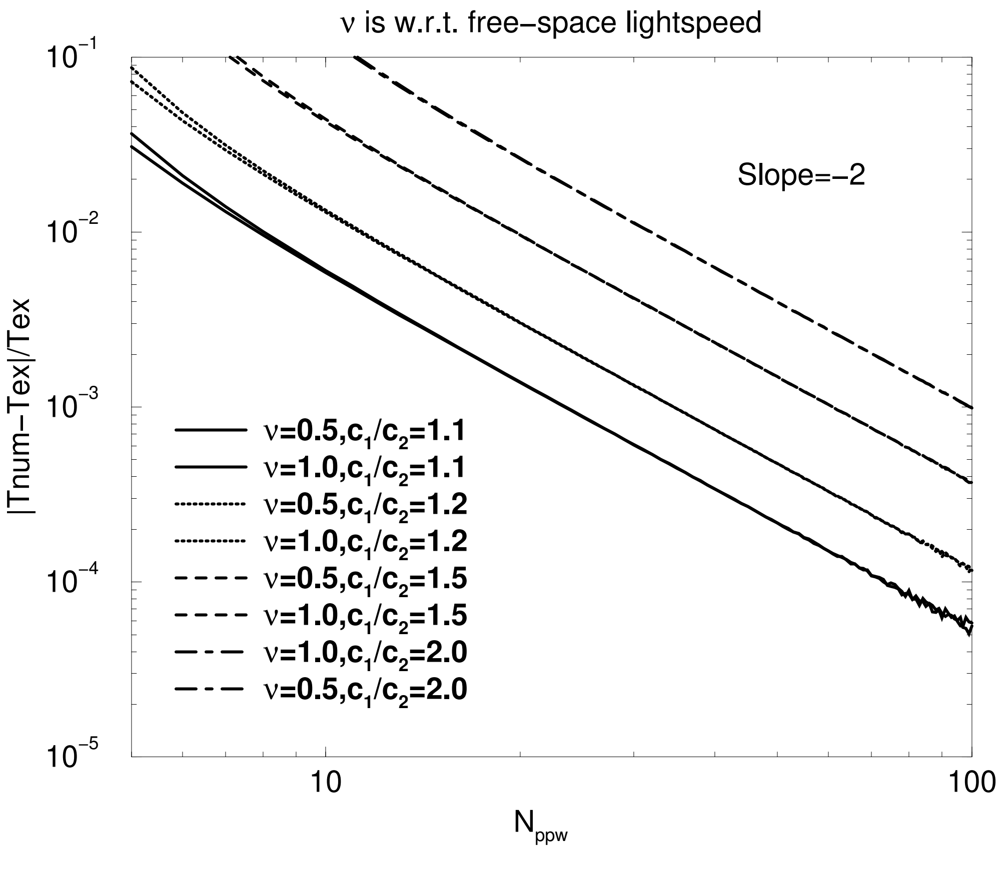
i.e., employing the "rule of thumb" $N_{ppw} \sim 10 - 20$ is a bad computational practice. For example, when waves propagate along $\theta = 0^o$ and $e_\phi = 6^o$, $N_{ppw} = 20$ is good only up to $J = 3$.

- Dielectric interface aligned with the grid

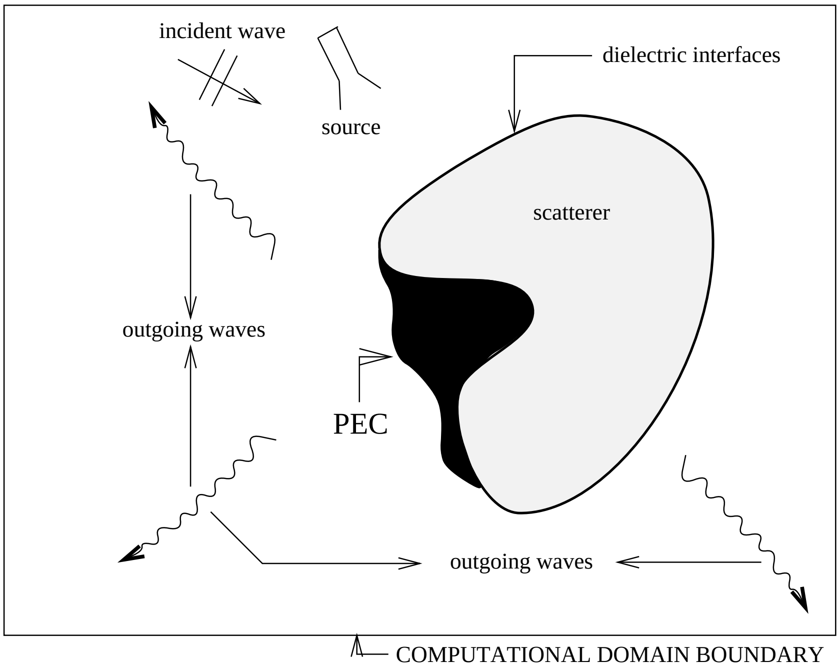


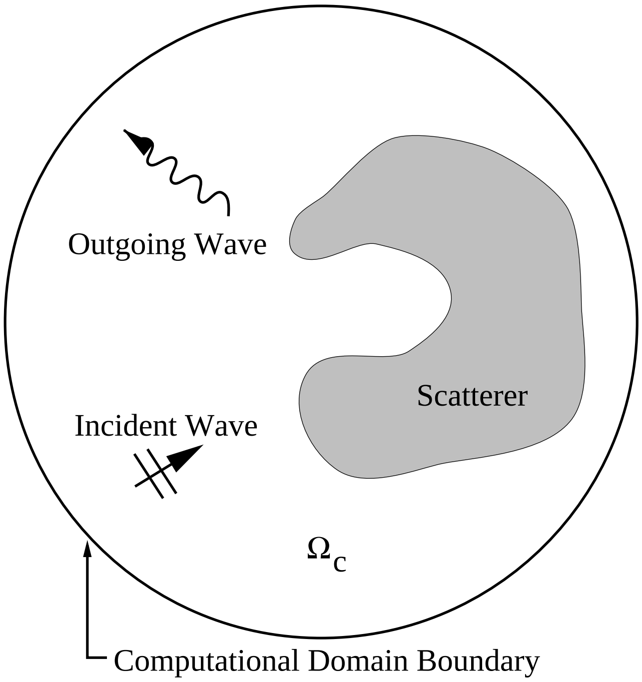
Local error at the interface node is $O(\Delta)$
$T.E. \sim \frac{1}{6} C_0^2 \Delta (\frac{C_1^2}{C_2^2} - 1) \frac{\partial^3 E(0,t)}{\partial X^3}$
where $C_0 = \sqrt{2} \frac{C_1 C_2}{C_1^2 + C_2^2}$ corresponds to using at the $x = 0$ node the average permittivity $(\epsilon_1 + \epsilon_2)/2$, $C_{1(2)} = 1/\sqrt{\epsilon_{1(2)} \mu_0}$ is the wave speed left(right) of the interface, and $E(0, t)$ is the electric field at x=0. Global error is second order. Any other choice for the permittivity at the node on $x = 0$ results in an $O(1)$ local error and a global loss of accuracy.

• Relative error in the transmission coefficient



- The absorbing boundary problem

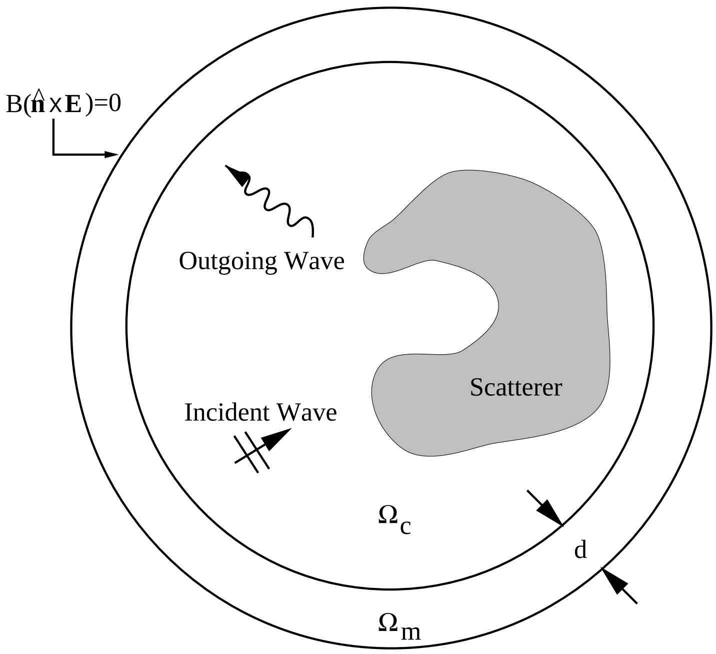




The computational domain is embedded in a background medium (may be dispersive) that extends to infinity but in a computation is truncated at a finite distance from scatterer.

The interior problem (hyperbolic or elliptic) is typically discretized with FEM, FDM, Pseudospectral, or Spectral methods.

On the computational domain boundary an approximation to the true radiation condition, $B_{app}(\hat{\mathbf{n}} \times \mathbf{E}) = 0$, is imposed on the tangential fields to provide boundary values for the interior algorithm.



- Reflectionless Absorbing Layers

An alternative to radiation boundary conditions (imposed on $\partial\Omega_c$) for absorbing outgoing waves from a scattering region involves surrounding the computational domain Ω_c with a wave absorbing layer, Ω_m, of thickness d. Ideally, the transition from the interior to the absorbing layer should not produce wave reflection while the fields that have penetrated into the layer should attenuate as they propagate outward. The boundary condition $B(\hat{\mathbf{n}} \times \mathbf{E}) = 0$ is used to truncate the layer and typically is the PEC condition.

- 1 Dimension

Consider the one-dimensional Maxwell system for $(x, t) \in (-\infty, \infty) \times [0, \infty)$

$$
\begin{aligned}
\mu \frac{\partial H}{\partial t} + \sigma^* H &= -\frac{\partial E}{\partial x} \\
\epsilon \frac{\partial E}{\partial t} + \sigma E &= -\frac{\partial H}{\partial x},
\end{aligned} \tag{1}
$$

where $\sigma = \sigma^* = 0$ for $x < 0$ and σ, $\sigma^* > 0$ for $x \geq 0$. System (1) models an electrically and magnetically lossy "material" (occupying $x \geq 0$) with constant wavefront speed $c_\infty = 1/\sqrt{\epsilon\mu}$, placed adjacent to free-space ($x < 0$) with wavefront speed $c = 1/\sqrt{\epsilon_0 \mu_0}$ (note: $c_\infty \leq c$). Using the notation $t_c = \epsilon/\sigma$, and $t_c^* = \mu/\sigma^*$ we compute the dispersion relation relevant to boundary value problems ($\omega \in \mathcal{R}$) in $x > 0$.

For a mode $e^{i(\omega t - kx)}$ it is

$$-\omega^2 + i\frac{\omega}{t_c} + i\frac{\omega}{t_c^*} + \frac{1}{t_c t_c^*} + c_\infty^2 k^2 = 0. \qquad (2)$$

Choosing "material" properties so that $t_c = t_c^*$ (the "PML condition") (2) reduces to

$$ik = \pm\tfrac{1}{c_\infty}(i\omega + \tfrac{1}{t_c}).$$

Left/right moving waves in this "material" travel slower than they do in $x < 0$, and decay exponentially in space at a rate that is independent of the frequency ω !

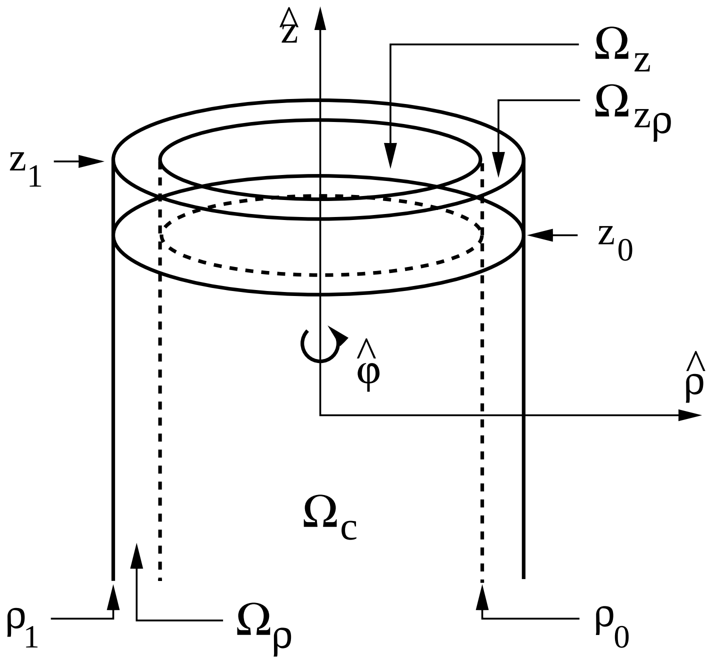
Is the interface reflectionless ?

If $\sqrt{\epsilon_0/\mu_0} = \sqrt{\epsilon/\mu}$ then (1), written as the system $\mathbf{u}_t + A\mathbf{u}_x + C\mathbf{u} = 0$ where $\mathbf{u} = (H, E)^T$, exhibits the following properties: $A = R\Lambda R^{-1}$ and $C = RDR^{-1}$, where $\Lambda = diag\{-c_\infty, c_\infty\}$ and $D = diag\{1/c_\infty t_c, -1/c_\infty t_c\}$, with R being the diagonalizer of the matrix A in the region $x < 0$ where the system is $\mathbf{u}_t + A_{x<0}\mathbf{u}_x = 0$ and $\Lambda_{x<0} = diag\{-c, c\} = R^{-1}A_{x<0}R$. Hence, the eigenvectors of A are preserved across $x = 0$, while its eigenvalues are reduced$\rightarrow$the interface at $x = 0$ will be reflectionless for any propagating wave impinging upon it from the left, and any propagating waves entering this "material" are slowed down ($c_\infty < c$) and damped independently of frequency.

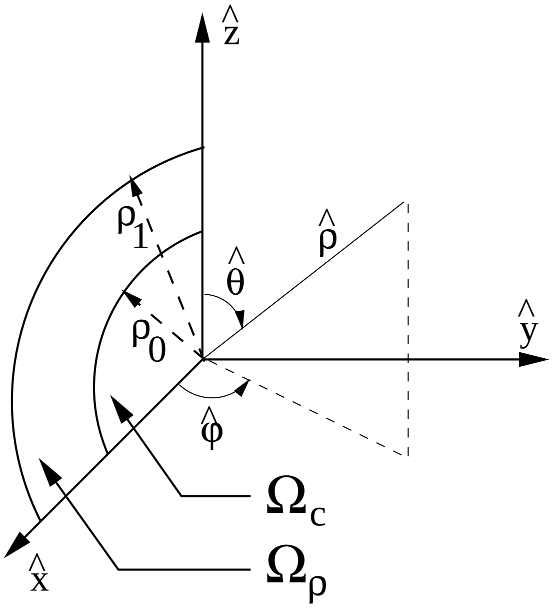
The region $x \geq 0$ can be terminated at $x = d > 0$ with any boundary condition (BC), e.g., Dirichlet or one of the popular ABCs, and the combination used as an absorbing boundary in a code that solves scattering problems in $x < 0$.

Appropriately setting d, t_c, and c_∞ can, in principle, make the boundary condition at $x = d$ invisible to waves in the interior $x < 0$, as any outgoing wave of amplitude E_0 that has entered the layer, and subsequently has reflected from the BC (e.g., Dirichlet) at $x = d$, will be further attenuated while propagating back towards $x = 0$ and will re-enter the computational domain with an exponentially small amplitude $\approx E_0 e^{-2d/c_\infty t_c}$.

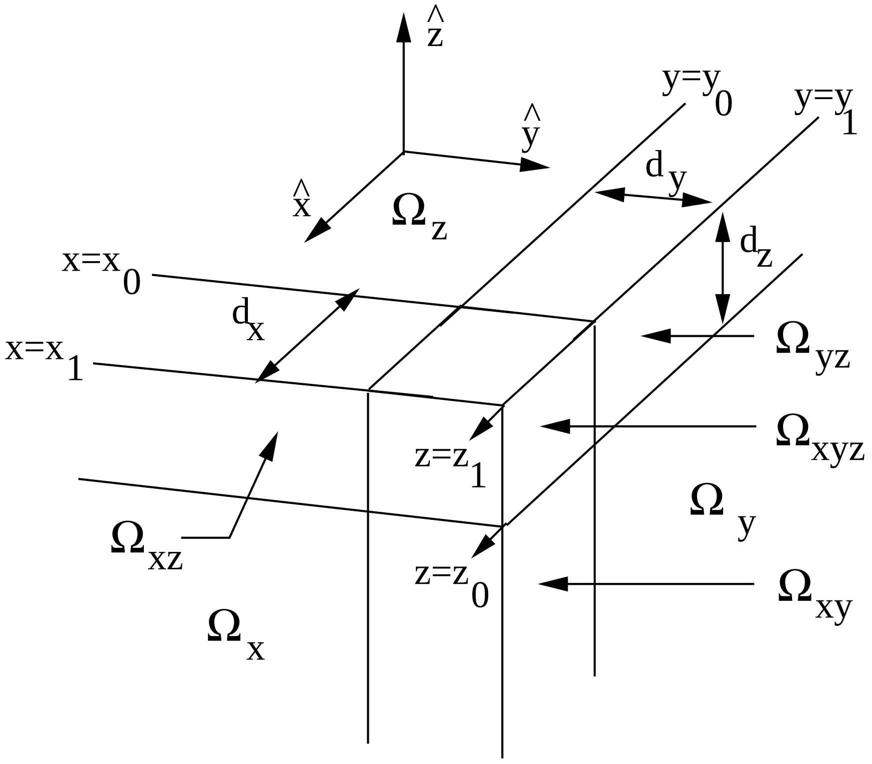
We note here that the order of accuracy and stability of a numerical scheme used in $x < 0$ can be maintained in $x > 0$ since the interior equations (which are (1) with $\sigma = \sigma^* = 0$ for $x < 0$) are modified in the layer by lower-order terms that can be appropriately time-centered in a discretization.



- Cylindrical (ρ, ϕ, z) coordinates

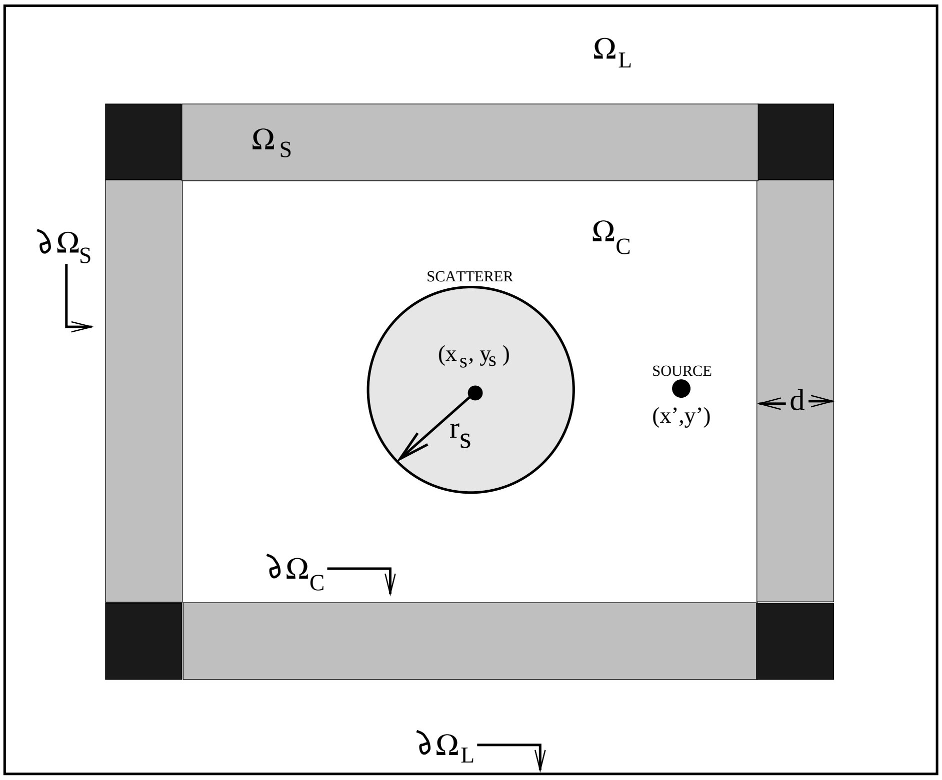


- Spherical (ρ, θ, ϕ) coordinates

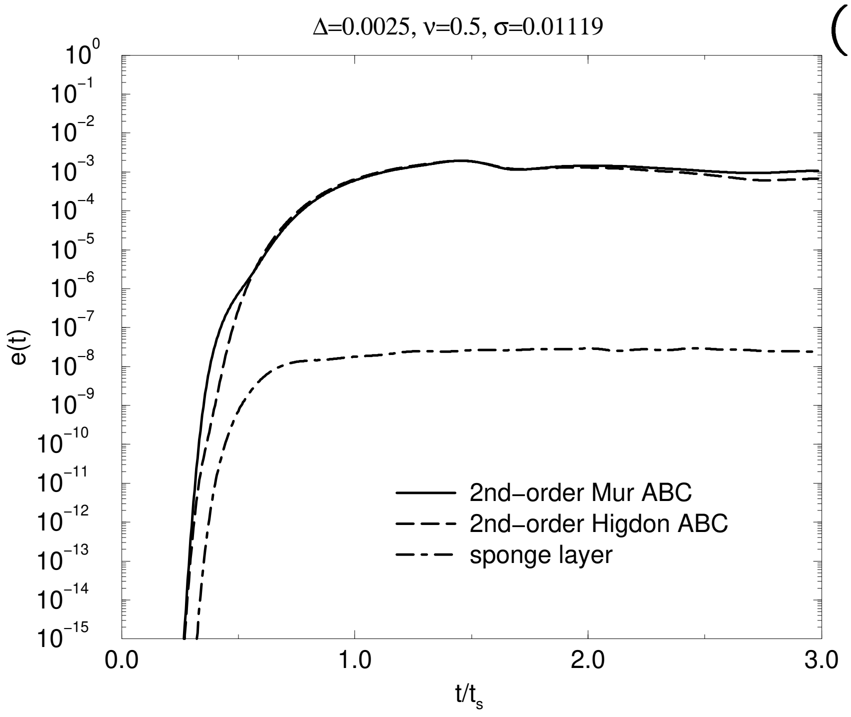


- Rectangular (x, y, z) coordinates

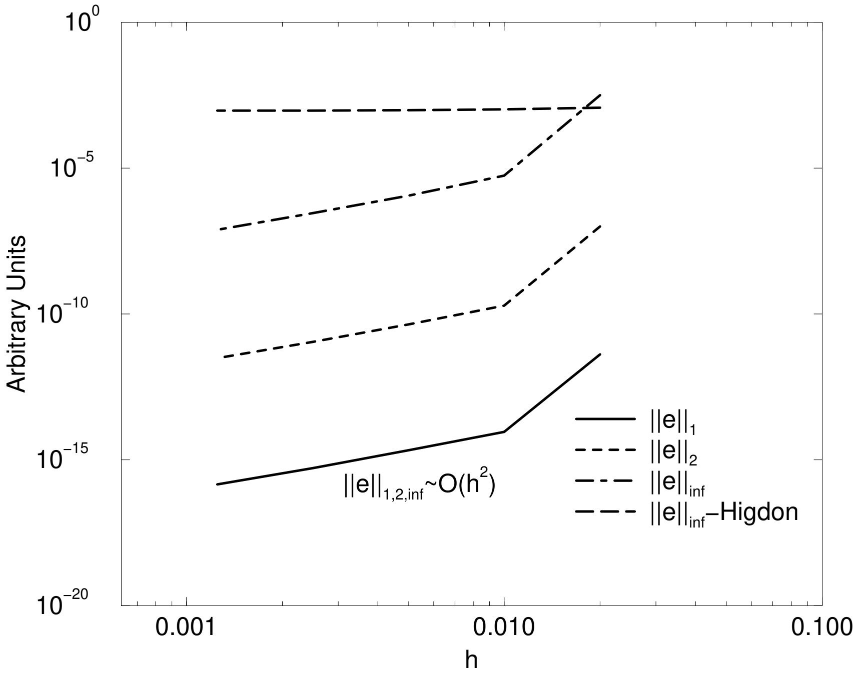
- Numerical experiment



(2-2) Scheme



Δ=0.0025, ν=0.5, σ=0.01119
e(t)
t/t_s
2nd−order Mur ABC
2nd−order Higdon ABC
sponge layer



Arbitrary Units
h
||e||_1
||e||_2
||e||_inf
||e||_inf−Higdon
||e||_{1,2,inf}~O(h^2)

—Absorbing boundaries and dispersion

Consider the 2D wave problem involving the B_1 absorbing operator in the left half-space:

$$\begin{aligned} u_{tt} - c^2(u_{xx} + u_{yy}) &= 0;\ x \in (-\infty, 0) \\ u_t + cu_x &= 0;\ x = 0. \end{aligned} \tag{3}$$

The dispersion relation for plane waves is $\omega = ck$. When

$$\begin{aligned} u(x,y,t) &= e^{i(kx\cos\theta + ky\sin\theta - \omega t)} \\ &+ R^c e^{i(-kx\cos\theta + ky\sin\theta - \omega t)} \end{aligned} \tag{4}$$

is substituted in the boundary condition at $x = 0$ we obtain the reflection coefficient

$$R^c(\theta) = -\frac{1 - \cos\theta}{1 + \cos\theta}. \tag{5}$$

Thus, the B_1 operator is an <u>*exact*</u> ABC for normally incident ($\theta = 0^o$) plane waves.

Next, we consider the standard, second-order accurate discretization of (3), with h being the mesh size and Δt the timestep. The numerical dispersion relation for discrete plane wave solutions is

$$\sin^2(\frac{\tilde{\omega}\Delta t}{2}) = \nu^2\{\sin^2(\frac{k\cos\theta h}{2})+\sin^2(\frac{k\sin\theta h}{2})\}, \tag{6}$$

where $\nu = c\Delta t/h$ is the Courant number ($\leq 1/\sqrt{2}$ for stability). Note that for $h,\ \Delta t \to 0$ we obtain $\tilde{\omega} \to \omega$.

It is easy to derive the reflection coefficient of the discrete B_1 operator:

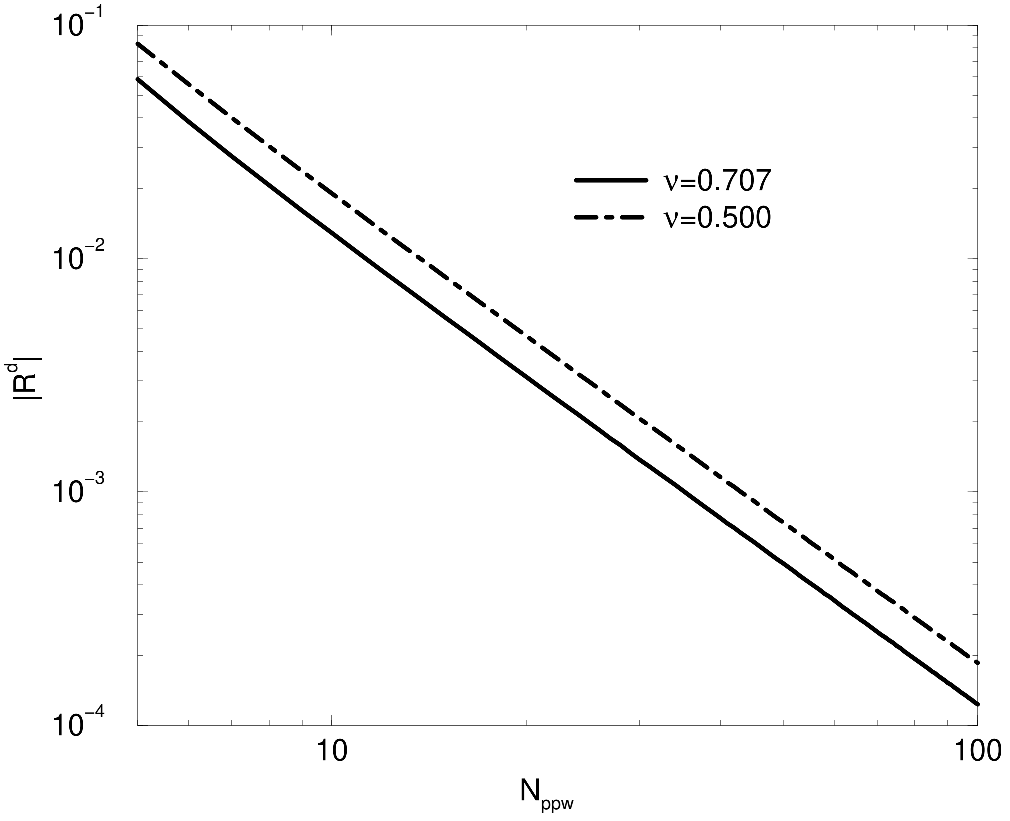
$$R^d(\theta, kh, \nu) = -e^{-ik\cos\theta h} \times \frac{\tan(\frac{\tilde{\omega}\Delta t}{2}) - \nu\tan(\frac{k\cos\theta h}{2})}{\tan(\frac{\tilde{\omega}\Delta t}{2}) + \nu\tan(\frac{k\cos\theta h}{2})}. \tag{7}$$

Making use of (6), and setting $\theta = 0^o$ (normally incident waves), reduces (7) to

$$R^d(0^o, kh, \nu) = -e^{-ikh} \times \frac{\cos(\frac{kh}{2}) - \sqrt{1-\nu^2\sin^2(\frac{kh}{2})}}{\cos(\frac{kh}{2}) + \sqrt{1-\nu^2\sin^2(\frac{kh}{2})}}. \tag{8}$$

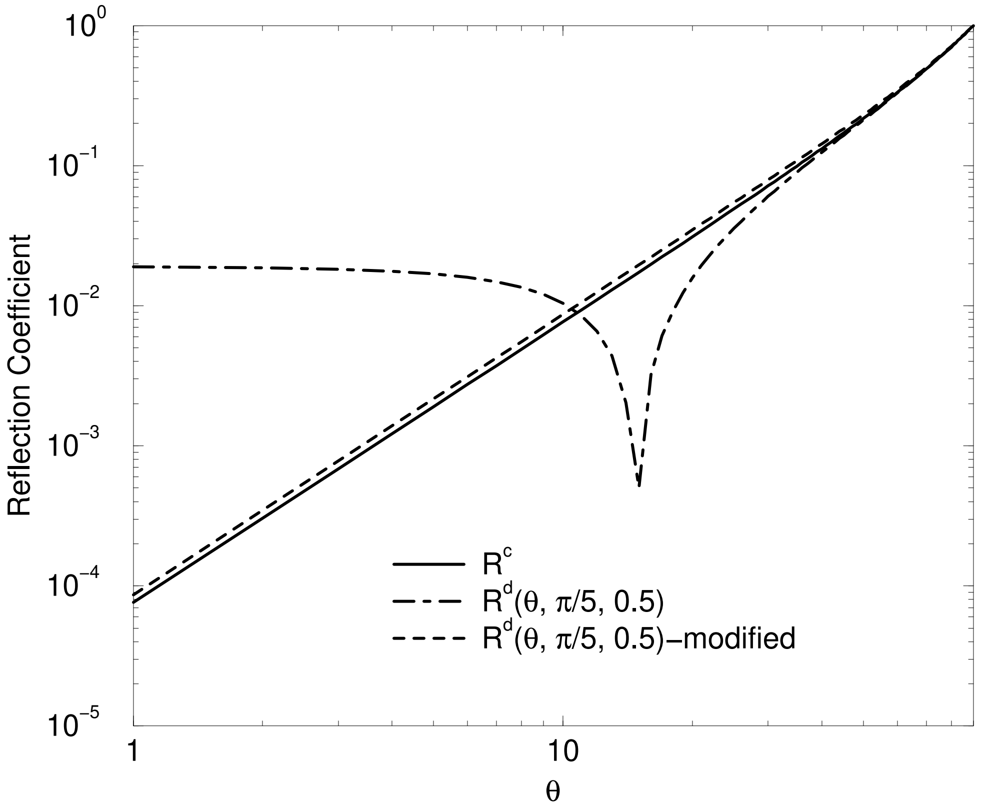
In contrast to (5), (8) shows the discrete B_1 operator is *not exact* for normally incident plane waves encountered in an actual computation.

Question: is this issue significant and, if it is, can it be fixed (i.e., can we restore the analytical zero-reflection property for $\theta = 0^o$ in discrete space) ?



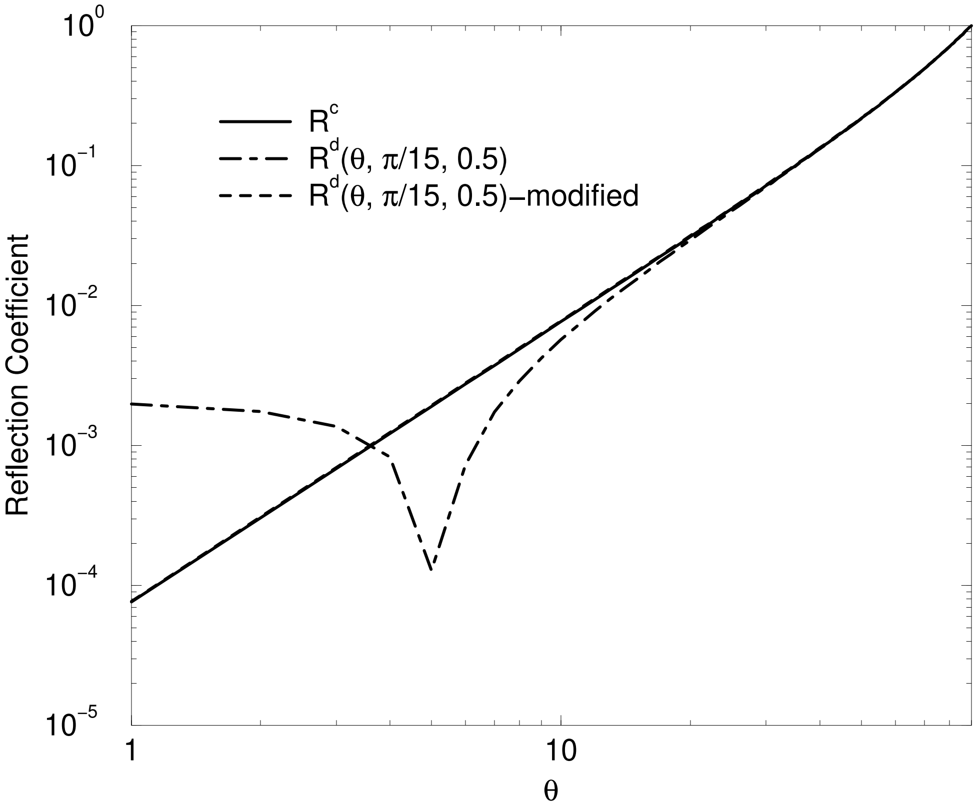
• A significant problem ?

Magnitude of the discrete reflection coefficient $R^d(0^o, kh, \nu)$ *vs.* $N_{ppw} = 2\pi/kh$ for two typical values of ν, one corresponding to the stability limit (when the interior scheme introduces the least dispersion) the other being a value used in actual computations in two dimensions.



• Can this problem be fixed ?

Magnitude of $R^d(0^o, kh, \nu)$ *vs.* θ for $N_{ppw} = 10$ and $\nu = 0.5$; the performance of the discrete ABC for plane waves near normal incidence is much worse than expected.



• Can this problem be fixed ?
Magnitude of $R^d(0^o, kh, \nu)$ *vs.* θ for $N_{ppw} = 30$ and $\nu = 0.5$; the performance of the discrete ABC for plane waves near normal incidence is still much worse (more than one order of magnitude) than expected.

The fix was effected by using in B_1 the numerical group velocity instead of the wavespeed c,

$$c_g(0^o, kh, \nu) = \frac{c \cdot \cos(\frac{kh}{2})}{\sqrt{1 - \nu^2 \sin^2(\frac{kh}{2})}}. \tag{9}$$

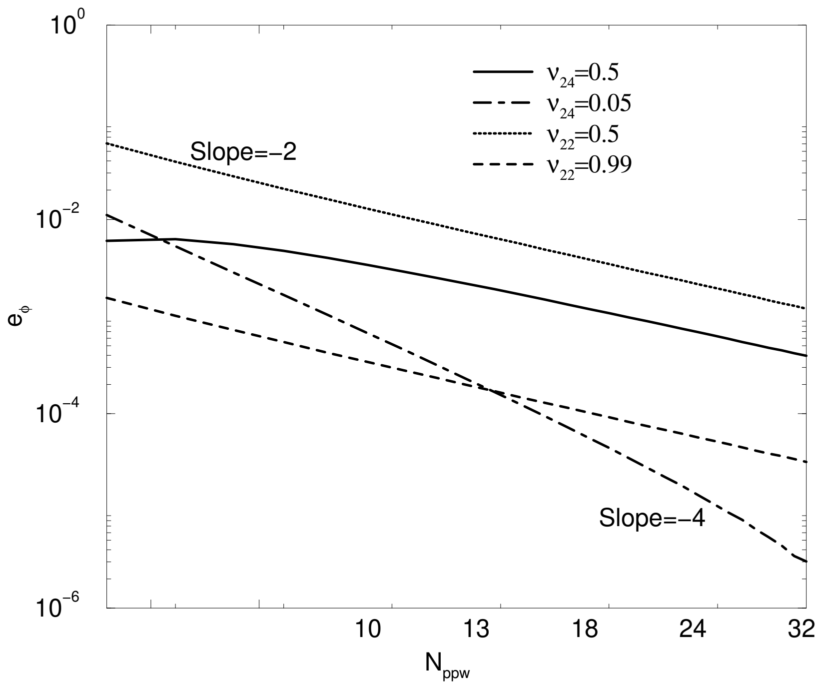
Then, $R^d(0^o, kh, \nu) = 0$ and R^c is fully recovered for all θ.

This approach can be applied to all discrete local and global ABC's and determine/correct their actual performance in a computation. For example, in the $M-$th order Higdon ABC

$$B_M = \prod_{q=1}^{M} (\frac{\partial}{\partial t} + \frac{c}{\alpha_q}\frac{\partial}{\partial x}); \;\; M \geq 2, \tag{10}$$

where $\alpha_q = \cos\theta_q$ are the cosines of the angles of perfect absorption for plane waves incident at an angle θ_q on the boundary at $x = 0$, the remedy is to use the interior scheme's group velocity $c_g(\theta_q, kh, \nu)$ instead of c in (10). Then, the analytical reflection coefficients will be observed in the discrete setting.

–A 4th-order scheme for CEM

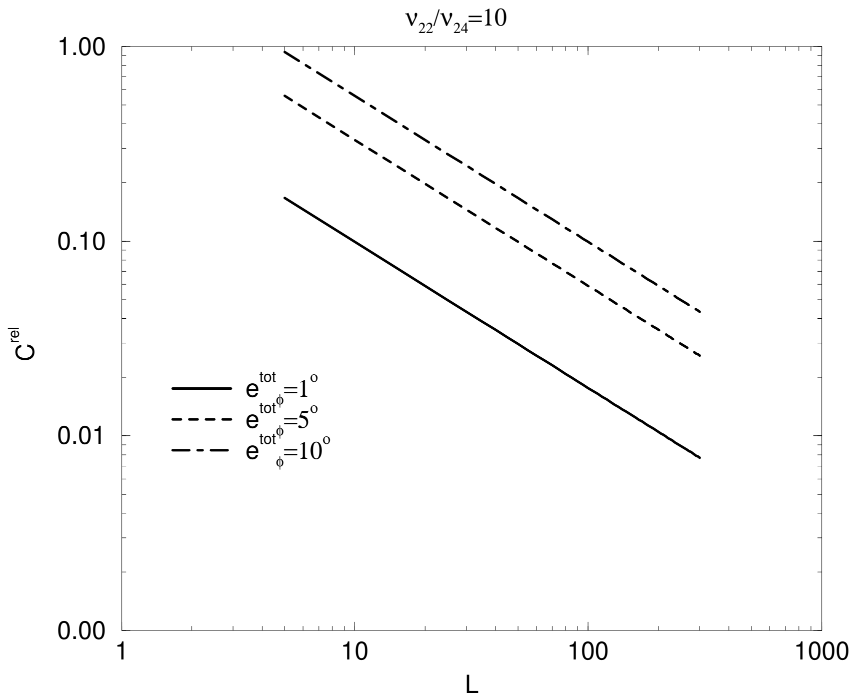


For small $\frac{\pi}{N_{ppw}}$ we have

$$N_{ppw} \sim (\frac{3}{20})^{\frac{1}{4}}\pi^{\frac{5}{4}}(sin^6\theta + cos^6\theta)^{\frac{1}{4}}(\frac{J}{e_\phi})^{\frac{1}{4}}$$

Note that now the N_{ppw} grows slower than in the send-order case. For waves propagating along $\theta = 0^o$ and $e_\phi = 6^o$, $N_{ppw} = 20$ is good up to $J = 22$ (recall, it was $J = 3$ with the send-order method).

• Relative computational cost

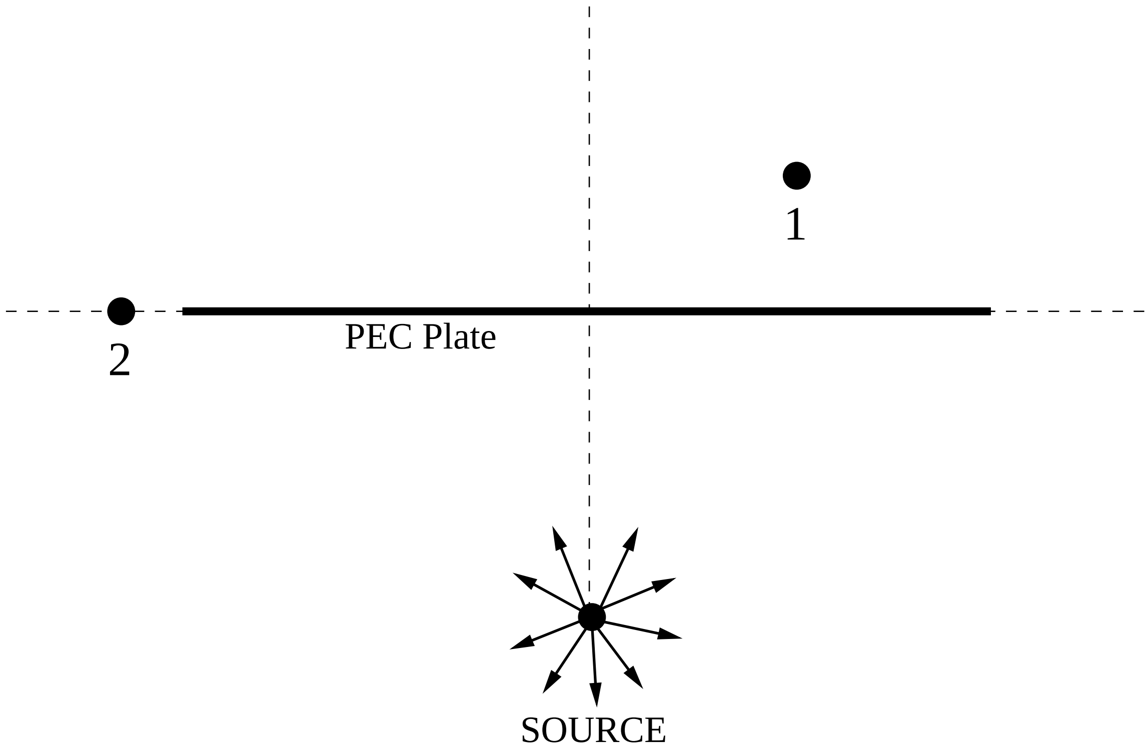


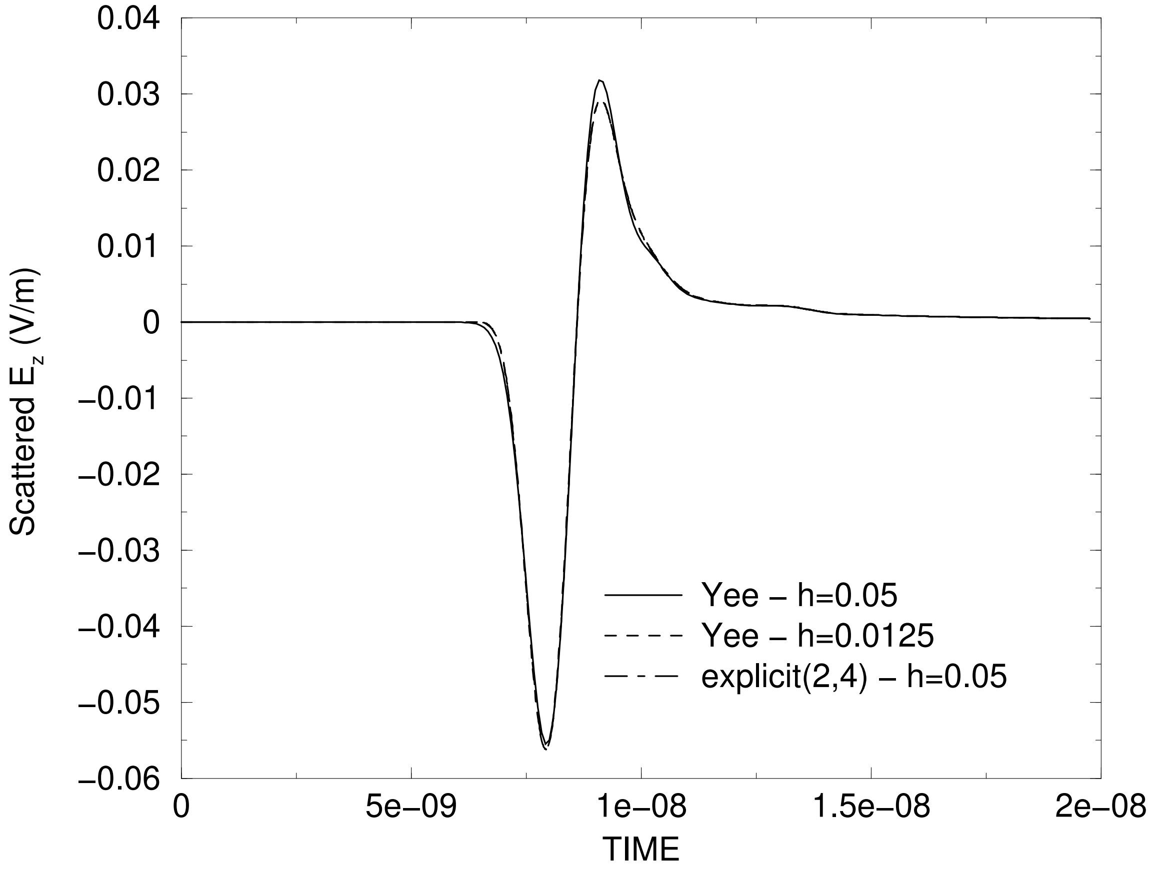
Taking into account the number of arithmetic operations per timestep, $\#OP/\Delta t$, and ν (for $\frac{\pi}{N_{ppw}} \ll 1$) we obtain

$$C^{rel} = \frac{C^{24}}{C^{22}} \sim 1.16 \times \frac{\nu 22}{\nu 24}(\frac{e_\phi}{L})^{\frac{3}{4}},$$

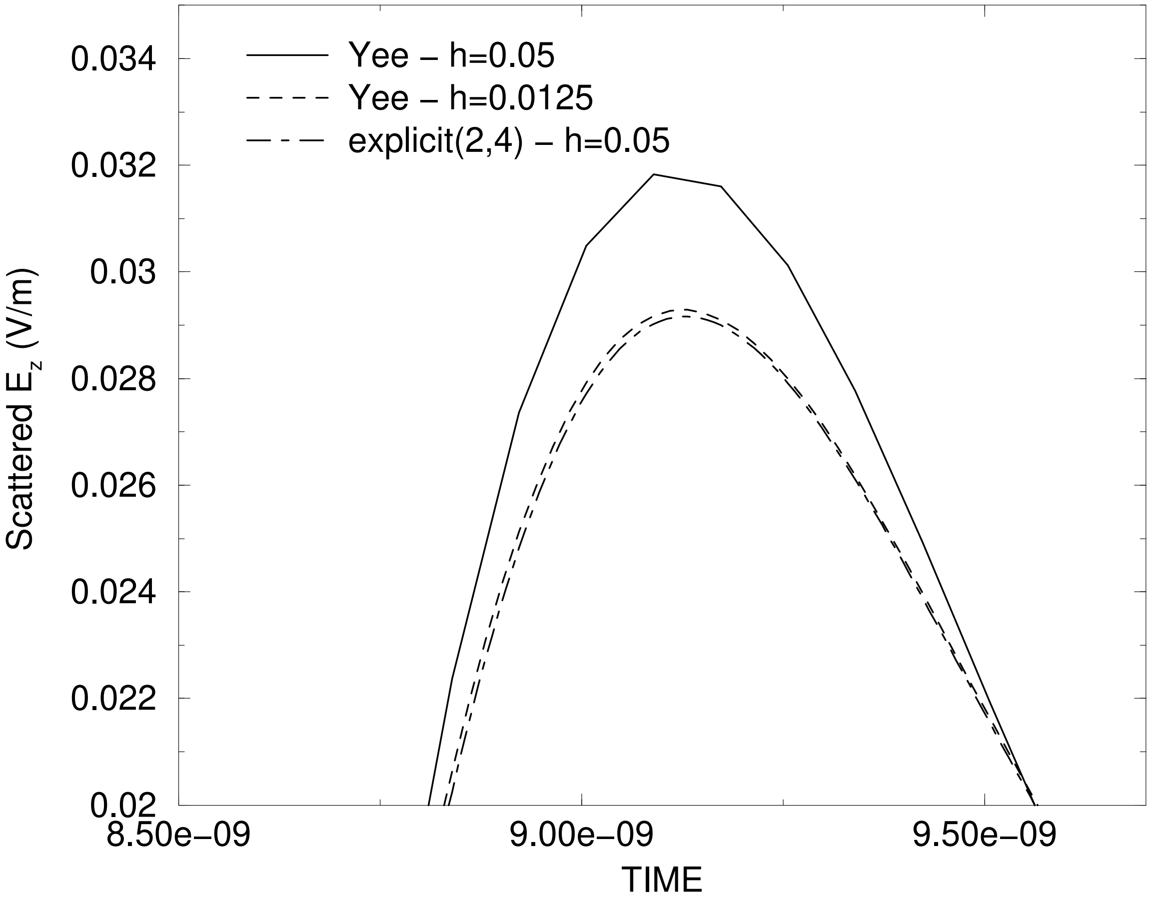
where L is domain size w.r.t. smallest wavelength (here, the smallest wavelength can also be thought to be that of the target boundary).

- An interesting problem

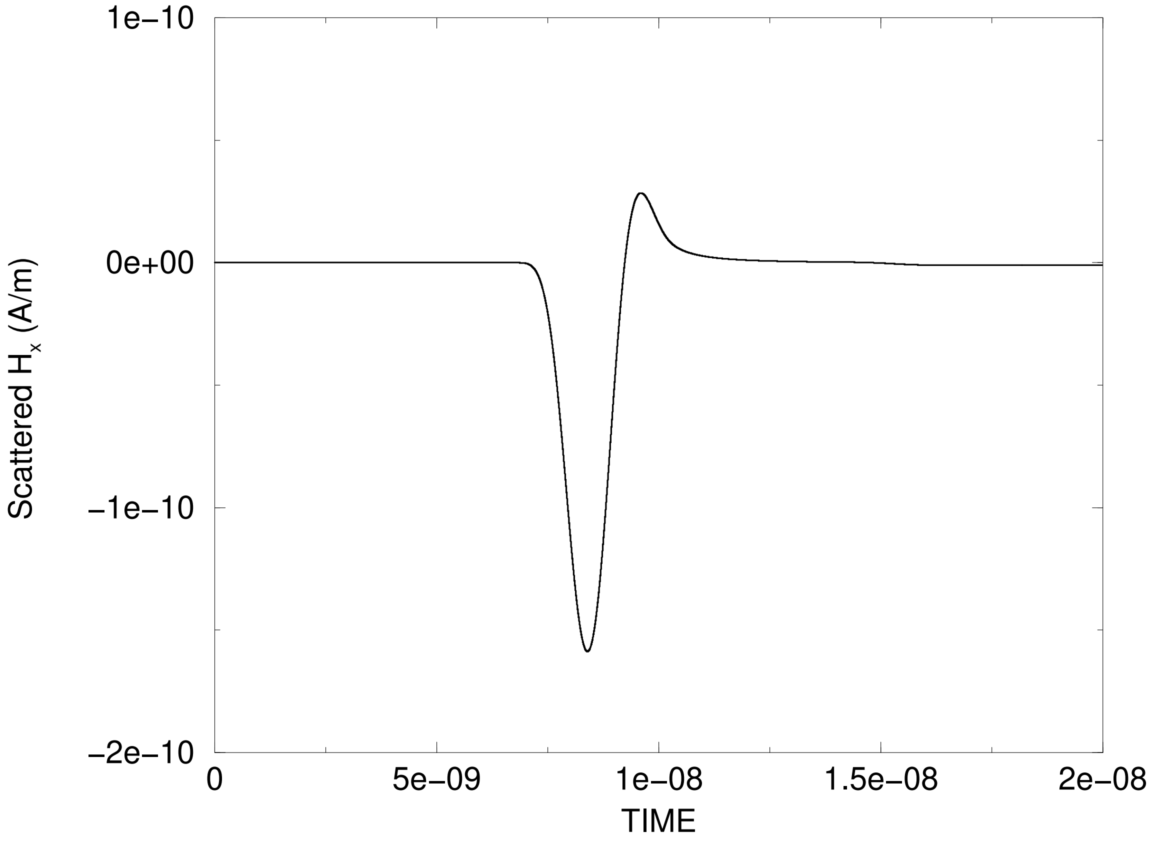




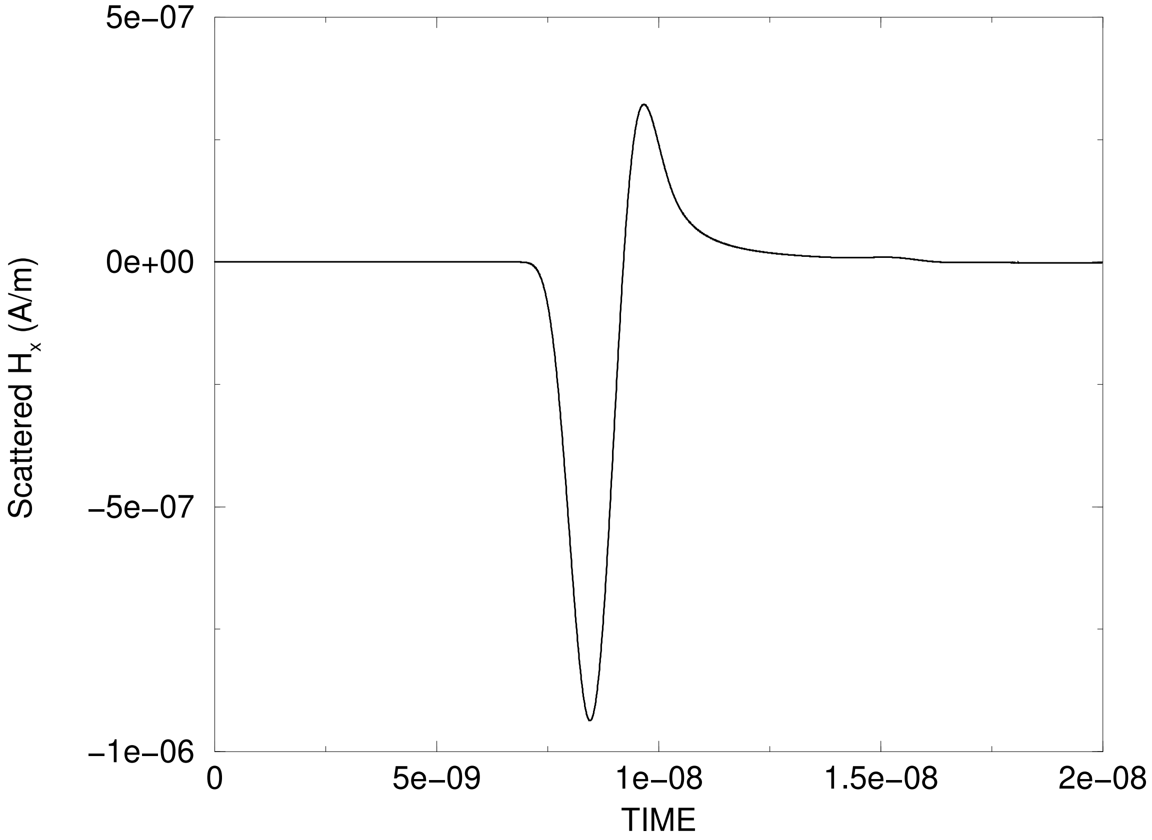
0.04
0.03
0.02
0.01
0
−0.01
−0.02
−0.03
−0.04
−0.05
−0.06
Scattered E_z (V/m)
0
5e−09
1e−08
1.5e−08
2e−08
TIME
Yee − h=0.05
Yee − h=0.0125
explicit(2,4) − h=0.05



Yee – h=0.05
Yee – h=0.0125
explicit(2,4) – h=0.05
Scattered E_z (V/m)
0.034
0.032
0.03
0.028
0.026
0.024
0.022
0.02
8.50e−09
9.00e−09
9.50e−09
TIME



1e−10
0e+00
−1e−10
−2e−10
Scattered H_x (A/m)
0
5e−09
1e−08
1.5e−08
2e−08
TIME



5e−07
0e+00
−5e−07
−1e−06
0
5e−09
1e−08
1.5e−08
2e−08
TIME
Scattered H_x (A/m)