TWO-STEP PERFECTLY MATCHED LAYER FOR ARBITRARY-ORDER PSEUDO-SPECTRAL ANALYTICAL TIME-DOMAIN METHODS

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CONTENTS

ONE-WAY ABCs DERIVED FROM DIFFERENTIAL EQUATIONS (by factoring the wave equation and allowing solution that permits only outgoing waves)	MATERIAL-BASED ABCs (use a layer of absorber material added at the outer boundary)

- Engquist and Majda (based on 1st or 2nd order of the Taylor series expansion of $\sqrt{(1-s^2)}$)
- Trefethen-Halpern $\sqrt{(1-s^2)} \approx \frac{P_n(s)}{Q_n(s)}$
- Higdon operator

■ MATCHED LAYER (ML)

(impedance of material boundary was matched to the free-space impedance only @ normal incidence)

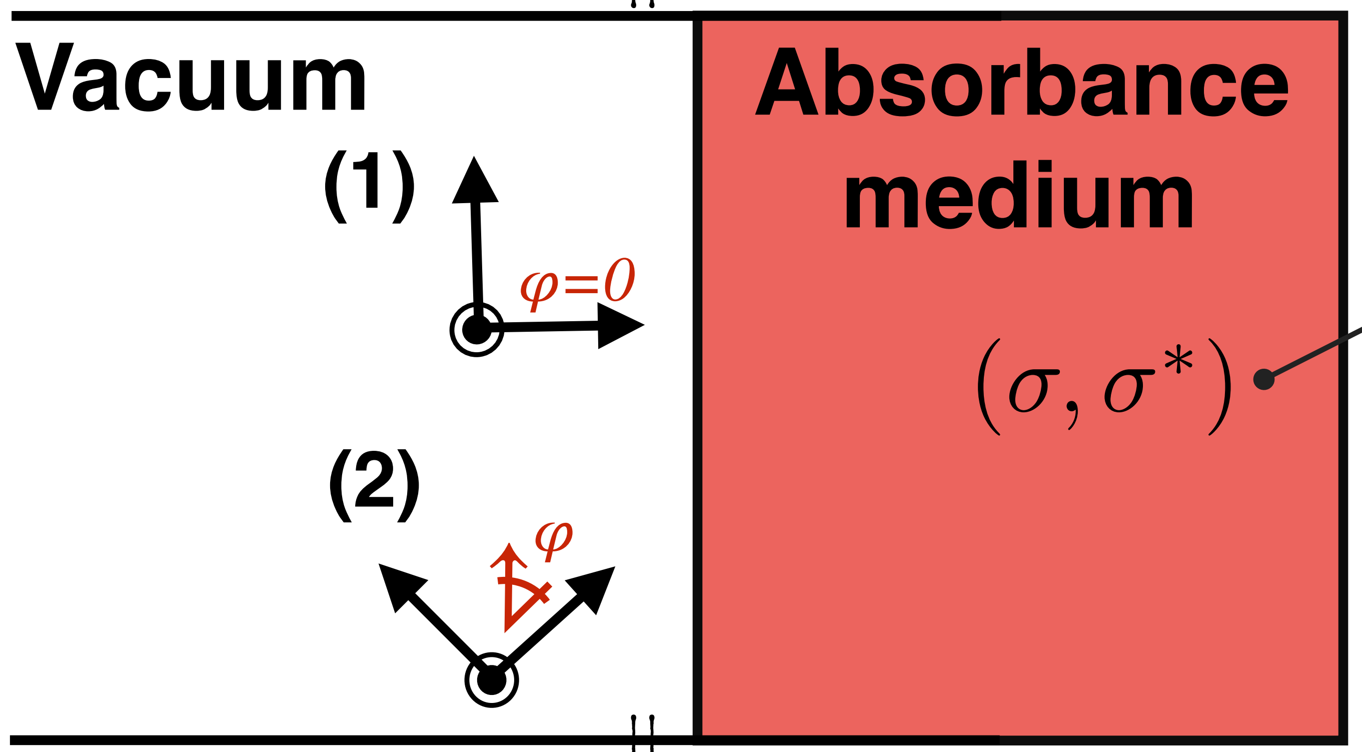
MATCHED LAYER (ML)

$$\varepsilon_0 \frac{\partial E_x}{\partial t} + \sigma E_x = \frac{\partial H_z}{\partial y}$$

$$\varepsilon_0 \frac{\partial E_y}{\partial t} + \sigma E_y = -\frac{\partial H_z}{\partial x}$$

$$\mu_0 \frac{\partial H_z}{\partial t} + \sigma^* H_z = \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}$$

Numerical electric/magnetic conductivities (σ, σ^*) ~ field decay in the absorbance medium



"Matching condition"

$$\frac{\sigma}{\varepsilon_0} = \frac{\sigma^*}{\mu_0}$$

(1) Normal incidence

$$R(0) = 0$$

(2) Oblique incidence

$$R(\varphi) = \frac{\cos(\varphi) - 1}{\cos(\varphi) + 1}$$

HISTORICAL REVIEW OF THE ABSORBING BOUNDARY CONDITIONS (ABCs)

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■ **MATCHED LAYER (ML)**

(impedance of material boundary was matched to the free-space impedance only @ normal incidence)

■ **PERFECTLY MATCHED LAYER (PML)**

(Splitting fields into orthogonal components)

J-P. Berenger, J. *Comput Phys.*, ***114***, *185-200* (1994)

PERFECTLY MATCHED LAYER (PML)

- Field components split
- Perfectly matched conditions

$$\frac{\sigma_x}{\varepsilon_0} = \frac{\sigma_x^*}{\mu_0} \;\&\; \frac{\sigma_y}{\varepsilon_0} = \frac{\sigma_y^*}{\mu_0}$$

$$\varepsilon_0 \frac{\partial E_x}{\partial t} + \sigma_y E_x = \frac{\partial (H_{zx} + H_{zy})}{\partial y}$$

$$\varepsilon_0 \frac{\partial E_y}{\partial t} + \sigma_x E_y = -\frac{\partial (H_{zx} + H_{zy})}{\partial x}$$

$$\mu_0 \frac{\partial H_{zx}}{\partial t} + \sigma_x^* H_{zx} = -\frac{\partial E_y}{\partial x}$$

$$\mu_0 \frac{\partial H_{zy}}{\partial t} + \sigma_y^* H_{zy} = \frac{\partial E_x}{\partial y}$$

$\forall \varphi : R(\varphi) = 0$ @ infinitesimal limit while FDTD/PSTD introduce residual reflections.

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(Splitting fields into orthogonal components)

J-P. Berenger, J. *Comput Phys., **114**, 185-200* (1994)

- Complex Coordinate Stretching PML (analytical continuation into the complex plane)
- Uniaxial PML (un-split PML)
- Nearly PML
- Convolutional PML
- **Asymmetric PML (APML)**

J-L. Vay, J. *Comput Phys., **183**, 367-399* (2011)

($\exists$ asymmetry in absorption rate for some setting of the extra coefficients)

ASYMMETRIC PERFECTLY MATCHED LAYER (APML)

$$
\begin{aligned}
\varepsilon_0 \frac{\partial E_x}{\partial t} + \sigma_y E_x &= \frac{c_y}{c}\frac{\partial H_z}{\partial y} + \cancel{\bar{\sigma}_y H_z}, \\
\varepsilon_0 \frac{\partial E_y}{\partial t} + \sigma_x E_y &= -\frac{c_x}{c}\frac{\partial H_z}{\partial x} + \cancel{\bar{\sigma}_x H_z}, \\
\mu_0 \frac{\partial H_{zx}}{\partial t} + \sigma_x^* H_{zx} &= -\frac{c_x^*}{c}\frac{\partial E_y}{\partial x} + \cancel{\bar{\sigma}_x^* E_y}, \\
\mu_0 \frac{\partial H_{zy}}{\partial t} + \sigma_y^* H_{zy} &= \frac{c_y^*}{c}\frac{\partial E_x}{\partial y} + \cancel{\bar{\sigma}_y^* E_x}, \\
H_z &= H_{zx} + H_{zy}.
\end{aligned}
$$

- if $\begin{aligned} c_x &= c_y = c_x^* = c_y^* = c \\ \bar{\sigma}_x &= \bar{\sigma}_y = \bar{\sigma}_x^* = \bar{\sigma}_y^* = 0, \end{aligned}$ $\Rightarrow$ **APML = PML**

Matching conditions

- if $\sigma_x/\epsilon_0 = \sigma_x^*/\mu_0$ and $\sigma_y/\epsilon_0 = \sigma_y^*/\mu_0$
  $c_x = c_x^*,\ c_y = c_y^*,\ \sigma_x = \sigma_x^*,\ \sigma_y = \sigma_y^*,$
  $\bar{\sigma}_x = \bar{\sigma}_x^*, \bar{\sigma}_y = \bar{\sigma}_y^*$
  $\Rightarrow \forall \varphi : R(\varphi) = 0$
  @ infinitesimal limit

With special choice of coefficients:

$$
\begin{aligned}
c_x^{(*)} &= c e^{-\sigma_x^{(*)}\Delta t} \frac{\sigma_x^{(*)}\Delta t}{1 - e^{-\sigma_x^{(*)}\Delta t}}, \\
c_y^{(*)} &= c e^{-\sigma_y^{(*)}\Delta t} \frac{\sigma_y^{(*)}\Delta t}{1 - e^{-\sigma_y^{(*)}\Delta t}},
\end{aligned}
$$

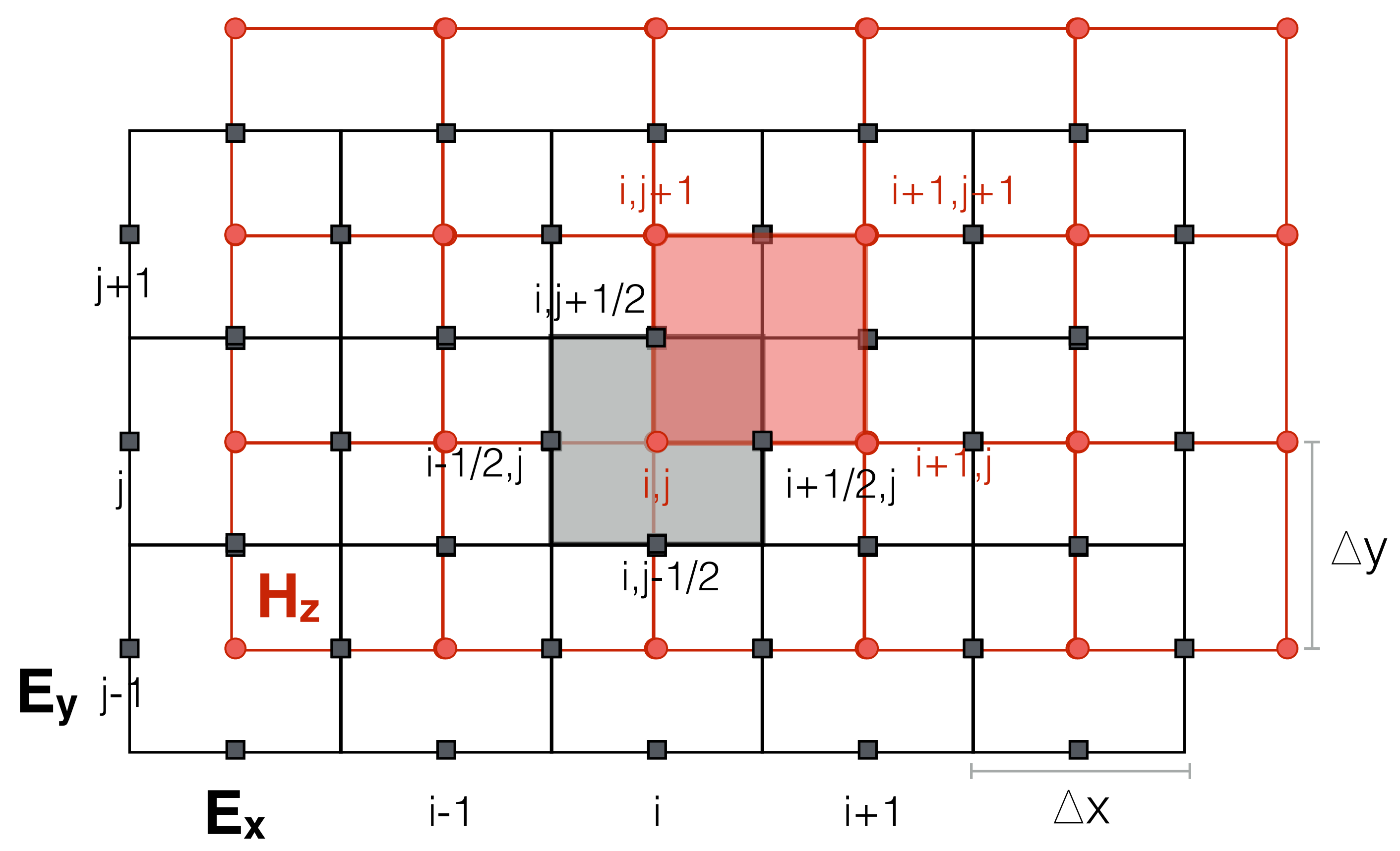
Note @ infinitisimal limit
$c_x^{(*)}, c_y^{(*)} \to c$ when $\Delta t \to 0$

J-L. Vay, *J. Comput Phys.*, ***183***, *367-399* (2011)

STANDARD 2ND-ORDER FDTD DISCRETIZATION (USING EXPONENTIAL TIME-STEPPING)

$$
\begin{aligned}
H_{zx}\big|^{n+1/2}_{i+1/2,j+1/2} &= e^{-\sigma^*_x \Delta t}\left[H_{zx}\big|^{n-1/2}_{i+1/2,j+1/2} - \frac{\Delta t}{\Delta x}\left(E_y\big|^{n}_{i+1,j+1/2} - E_y\big|^{n}_{i,j+1/2}\right)\right],\\
H_{zy}\big|^{n+1/2}_{i+1/2,j+1/2} &= e^{-\sigma^*_y \Delta t}\left[H_{zy}\big|^{n-1/2}_{i+1/2,j+1/2} + \frac{\Delta t}{\Delta y}\left(E_x\big|^{n}_{i+1/2,j+1} - E_x\big|^{n}_{i+1/2,j}\right)\right],\\
E_x\big|^{n+1}_{i+1/2,j} &= e^{-\sigma_y \Delta t}\left[E_x\big|^{n}_{i+1/2,j} + \frac{\Delta t}{\Delta y}\left(H_z\big|^{n+1/2}_{i+1/2,j+1/2} - H_z\big|^{n+1/2}_{i+1/2,j-1/2}\right)\right],\\
E_y\big|^{n+1}_{i,j+1/2} &= e^{-\sigma_x \Delta t}\left[E_y\big|^{n}_{i,j+1/2} - \frac{\Delta t}{\Delta x}\left(H_z\big|^{n+1/2}_{i+1/2,j+1/2} - H_z\big|^{n+1/2}_{i-1/2,j+1/2}\right)\right].
\end{aligned}
\qquad (*)
$$

2D spatial arrangement of the **E** an **H** field components on "Yee" staggered in space and time grid



TWO-STEP TIME-STAGGERED PML ("PML-2SS")

Equivalently :

(*) $\Leftrightarrow$

$$
\begin{aligned}
H^*_{zx}\big|^{n+1/2}_{i+1/2,j+1/2} &= H_{zx}\big|^{n-1/2}_{i+1/2,j+1/2} - \frac{\Delta t}{\Delta x}\left(E_y\big|^n_{i+1,j+1/2} - E_y\big|^n_{i,j+1/2}\right),\\
H^*_{zy}\big|^{n+1/2}_{i+1/2,j+1/2} &= H_{zy}\big|^{n-1/2}_{i+1/2,j+1/2} + \frac{\Delta t}{\Delta y}\left(E_x\big|^n_{i+1/2,j+1} - E_x\big|^n_{i+1/2,j}\right),\\
H_{zx}\big|^{n+1/2}_{i+1/2,j+1/2} &= e^{-\sigma^*_x \Delta t} H^*_{zx}\big|^{n+1/2}_{i+1/2,j+1/2},\\
H_{zy}\big|^{n+1/2}_{i+1/2,j+1/2} &= e^{-\sigma^*_y \Delta t} H^*_{zy}\big|^{n+1/2}_{i+1/2,j+1/2},\\
E^*_x\big|^{n+1}_{i+1/2,j} &= E_x\big|^n_{i+1/2,j} + \frac{\Delta t}{\Delta y}\left(H_z\big|^{n+1/2}_{i+1/2,j+1/2} - H_z\big|^{n+1/2}_{i+1/2,j-1/2}\right),\\
E^*_y\big|^{n+1}_{i,j+1/2} &= E_y\big|^n_{i,j+1/2} - \frac{\Delta t}{\Delta x}\left(H_z\big|^{n+1/2}_{i+1/2,j+1/2} - H_z\big|^{n+1/2}_{i-1/2,j+1/2}\right),\\
E_x\big|^{n+1}_{i+1/2,j} &= e^{-\sigma_y \Delta t} E^*_x\big|^{n+1}_{i+1/2,j},\\
E_y\big|^{n+1}_{i,j+1/2} &= e^{-\sigma_x \Delta t} E^*_y\big|^{n+1}_{i,j+1/2}.
\end{aligned}
$$

TWO-STEP TIME-CENTERED PML ("PML-2CS")

$$
\begin{aligned}
H^*_{zx}\big|^{n+1/2}_{i+1/2,j+1/2} &= H_{zx}\big|^{n}_{i+1/2,j+1/2} - 0.5\frac{\Delta t}{\Delta x}\left(E_y\big|^{n}_{i+1,j+1/2} - E_y\big|^{n}_{i,j+1/2}\right),\\
H^*_{zy}\big|^{n+1/2}_{i+1/2,j+1/2} &= H_{zy}\big|^{n}_{i+1/2,j+1/2} + 0.5\frac{\Delta t}{\Delta y}\left(E_x\big|^{n}_{i+1/2,j+1} - E_x\big|^{n}_{i+1/2,j}\right),\\
E^*_{x}\big|^{n+1}_{i+1/2,j} &= E_{x}\big|^{n}_{i+1/2,j} + \frac{\Delta t}{\Delta y}\left(H^*_z\big|^{n+1/2}_{i+1/2,j+1/2} - H^*_z\big|^{n+1/2}_{i+1/2,j-1/2}\right),\\
E^*_{y}\big|^{n+1}_{i,j+1/2} &= E_{y}\big|^{n}_{i,j+1/2} - \frac{\Delta t}{\Delta x}\left(H^*_z\big|^{n+1/2}_{i+1/2,j+1/2} - H^*_z\big|^{n+1/2}_{i-1/2,j+1/2}\right),\\
H^*_{zx}\big|^{n+1}_{i+1/2,j+1/2} &= H^*_{zx}\big|^{n+1/2}_{i+1/2,j+1/2} - 0.5\frac{\Delta t}{\Delta x}\left(E^*_y\big|^{n+1}_{i+1,j+1/2} - E^*_y\big|^{n}_{i,j+1/2}\right),\\
H^*_{zy}\big|^{n+1}_{i+1/2,j+1/2} &= H^*_{zy}\big|^{n+1/2}_{i+1/2,j+1/2} + 0.5\frac{\Delta t}{\Delta y}\left(E^*_x\big|^{n}_{i+1/2,j+1} - E^*_x\big|^{n}_{i+1/2,j}\right),\\
H_{zx}\big|^{n+1}_{i+1/2,j+1/2} &= e^{-\sigma^*_x\Delta t}H^*_{zx}\big|^{n+1}_{i+1/2,j+1/2},\\
H_{zy}\big|^{n+1}_{i+1/2,j+1/2} &= e^{-\sigma^*_y\Delta t}H^*_{zy}\big|^{n+1}_{i+1/2,j+1/2},\\
E_{x}\big|^{n+1}_{i+1/2,j} &= e^{-\sigma_y\Delta t}E^*_{x}\big|^{n+1}_{i+1/2,j},\\
E_{y}\big|^{n+1}_{i,j+1/2} &= e^{-\sigma_x\Delta t}E^*_{y}\big|^{n+1}_{i,j+1/2}.
\end{aligned}
$$

NOVEL TWO-STEP PML FORMULATION

At each time step, the field components **E** and **H** are updated in the following order:

(1) SOLVE MAXWELL'S EQUATIONS IN VACUUM OVER ONE TIME STEP

(2) MULTIPLY UPDATED FIELD COMPONENTS BY CORRESPONDING PML'S DAMPING COEFFICIENTS $e^{-\sigma_u^{(*)}\Delta t}$

⚠ Novel two-step technique is very versatile and can be used as is with any Maxwell solver for step (1) and **without re-writing discretized equations for the PMLs.**

DISCRETIZATION – EXTENSION TO HIGH-ORDER FDTD, PSTD & PSATD

- HIGH-ORDER FDTD DISCRETIZATION
- PSTD DISCRETIZATION
- PSATD DISCRETIZATION (under assumption that source terms are constant over one time interval ⇒ Maxwell's equation can be integrated analytically one time step)

DISPERSION RELATION ANALYSIS OF THE PML, PML-2SS AND PML-2SC

Dispersion relation equation as quadratic equation $e^{2i\omega\Delta t} + be^{i\omega\Delta t} + c = 0$:

$$\omega(k) = -\frac{i}{\Delta t}\ln\Big(\frac{-b \pm \sqrt{b^2 - 4c}}{2}\Big).$$

Note only positive sign solution has been considered, while the negative sign (``parasitic") solution has been disregard

PML: $\alpha^{(*)} = e^{-\sigma^{(*)}\Delta t}$, $\beta^{(*)} = c\frac{1-e^{-\sigma^{(*)}\Delta t}}{\sigma^{(*)}\Delta x}$; $b = -(\alpha + \alpha^*) - \beta\beta^*\chi_{km}$, $c = \alpha\alpha^*$;

PML-2SS: $\alpha^{(*)} = e^{-\sigma^{(*)}\Delta t}$, $\beta^{(*)} = c\frac{\Delta t}{\Delta x}$; $b = -(\alpha + \alpha^*) - \beta\beta^*\chi_{km}$, $c = \alpha\alpha^*$;

PML-2CS: $\alpha^{(*)} = e^{-\sigma^{(*)}\Delta t}$, $\beta^{(*)} = c\frac{\Delta t}{\Delta x}$; $b = -(\alpha + \alpha^*)(1 + \beta\beta^*\chi_{km}/2)$, $c = \alpha\alpha^*$

$$\chi_{km} = \sum_{k=1}^{p/2}\sum_{m=1}^{p/2} c_k^p c_m^p\big[e^{-ik\Delta x(k+m-1)} - e^{-ik\Delta x(k-m)} - e^{ik\Delta x(k-m)} + e^{ik\Delta x(k+m-1)}\big]$$

DISPERSION RELATION ANALYSIS OF THE PML, PML-2SS AND PML-2SC $(c\Delta t = 0.4\Delta x)$

$\sigma = \sigma^* = 0.64$

2ND ORDER

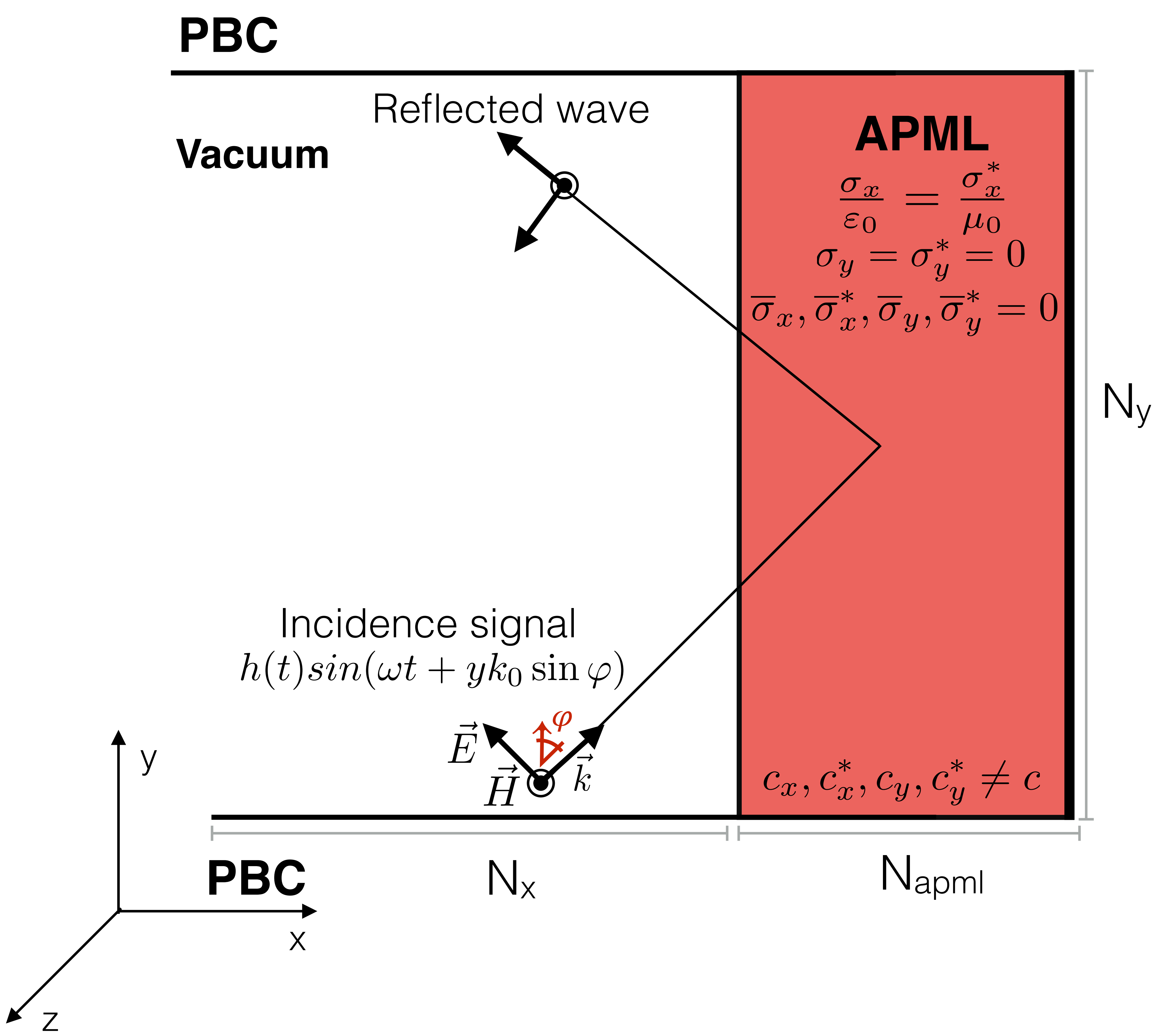
$\sigma = \sigma^* = 5.76$

- Re[ω(k)]PML-2SC ≈ CONST when σ ↗
- Re[ω(k)]PML-2SS ≠ CONST when σ ↗ (by construction)
- Im[ω(k)]PML/PML-2SS/PML-2SC ↗ when σ ↗ ~ σ

Re[ω(k)] ~ speed of waves
Im[ω(k)] ~ damping of waves

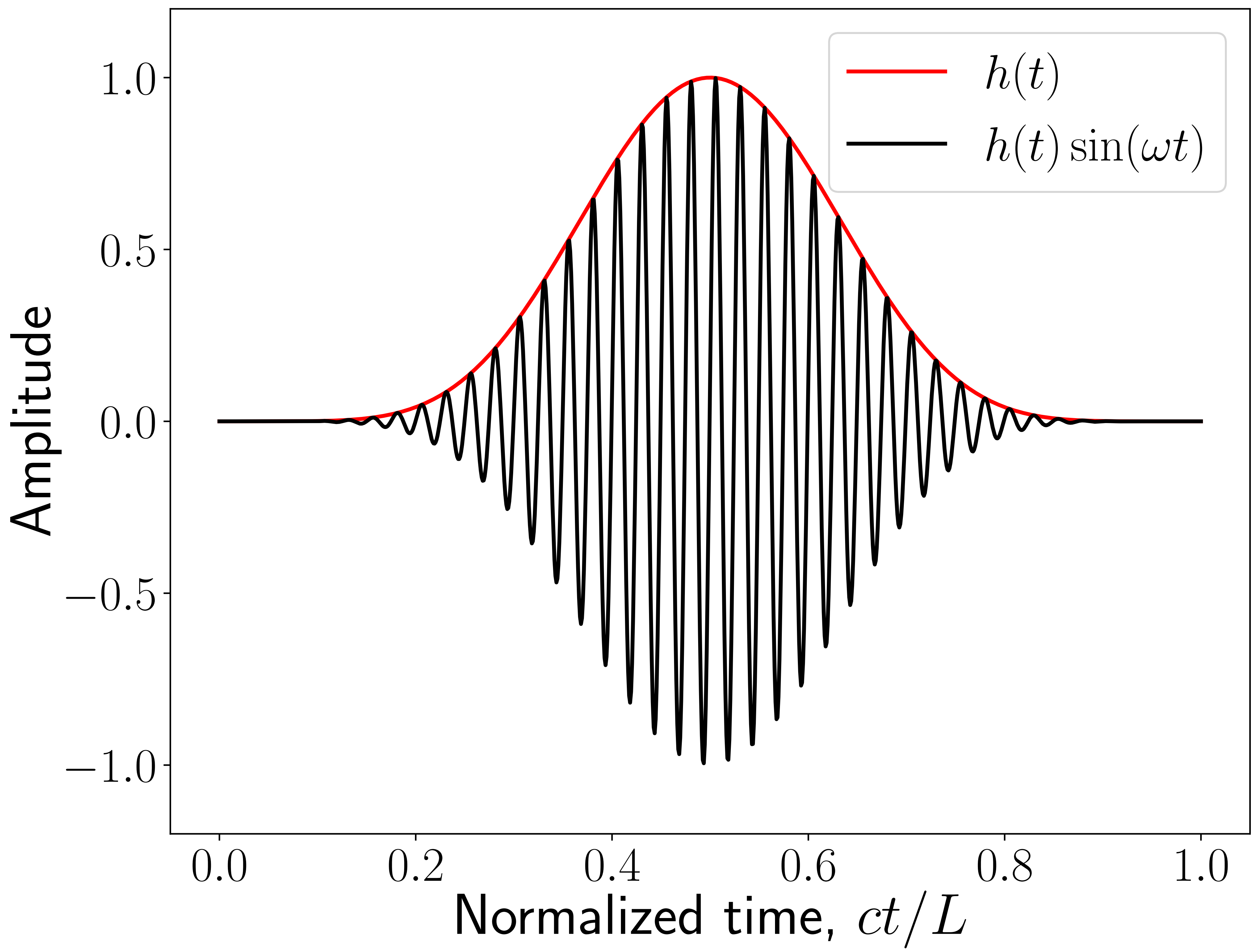
SIMULATION PARAMETERS

Schematic 2D representation of the TE plane-wave striking right-hand APML



Harris function (as temporal profile)

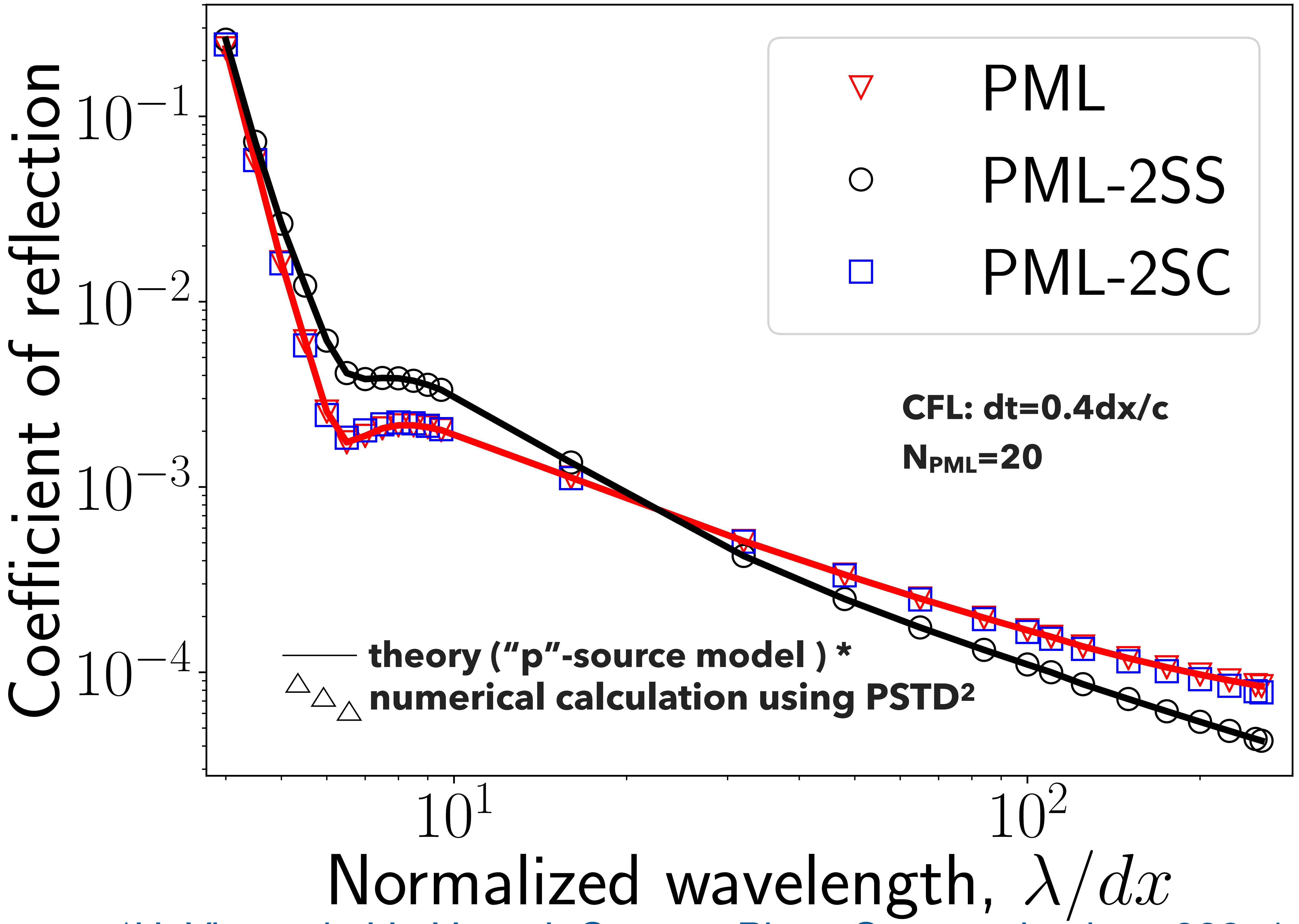
$$h(t) = \begin{cases} \frac{1}{32}\Big(10 - 15\cos(\frac{2\pi ct}{L}) + 6\cos(\frac{4\pi ct}{L}) - \cos(\frac{6\pi ct}{L})\Big), & \text{if } 0 < \frac{ct}{L} < 1 \\ 0, & \text{otherwise.} \end{cases}$$



COMPARISON OF THE REFLECTION COEFFICIENT @ NORMALLY INCIDENT PLANE WAVE

Numerical & analytical results confirms predictions made by numerical dispersion analysis:

- ✔ $R_{PML-2SC} \sim R_{PML}$ @ all wavelength
- ✔ $R_{PML-2SS}$ differs from R_{PML} (higher R @ short wavelength & lower R @ long wavelength)



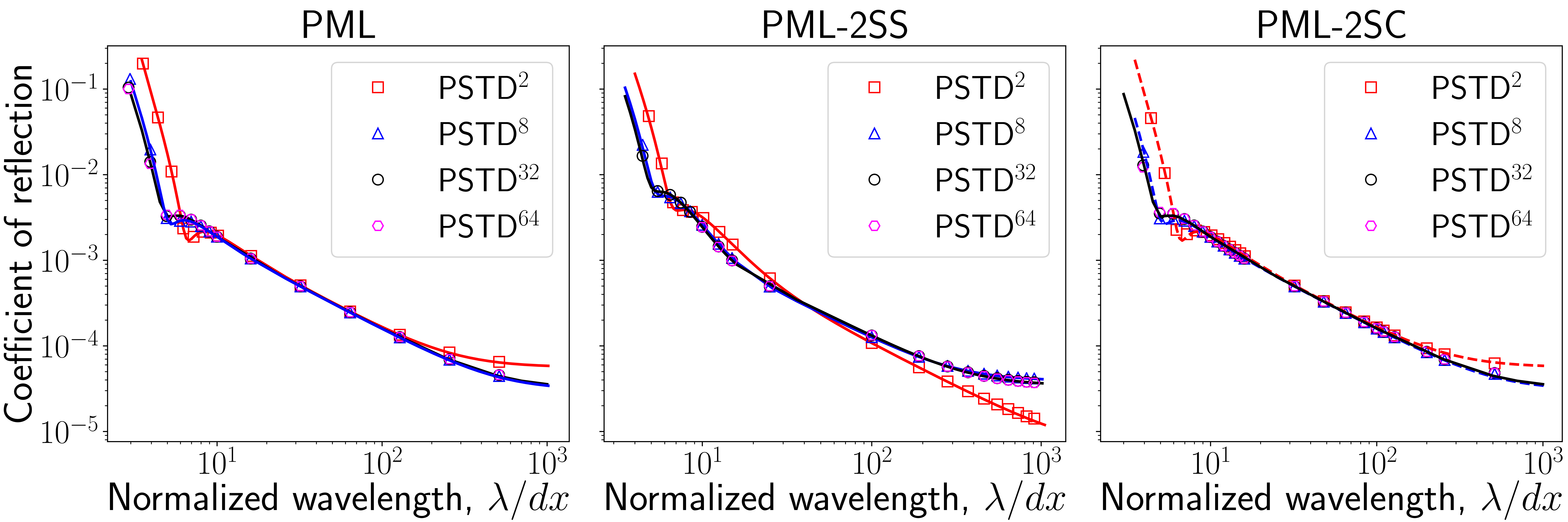
*H. Vincenti, J.L. Vay , J. Comput Phys. Communications 200, 147-167, (2016)

PML, PML-2SS, PML-2SC: PSTD^p (p=2,8,32,64) VS. THEORY

@ NORMALLY INCIDENT PLANE-WAVE

CFL: dt=0.4dx/c

N_{PML}=20

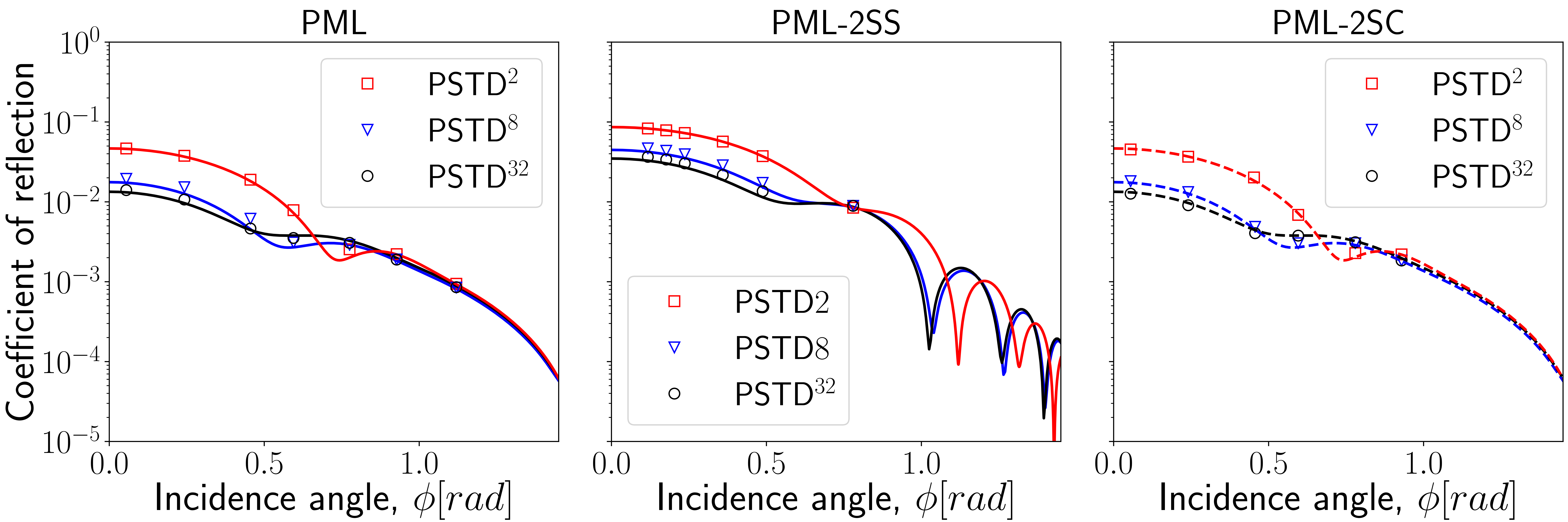


—— theory (“p”-source model)

△△△ numerical calculation using PSTD^p

PML, PML-2SS, PML-2SC: PSTD^p (p=2,8,32,64) VS. THEORY

@ OBLIQUE INCIDENT PLANE-WAVE @ $\lambda/dx = 4$

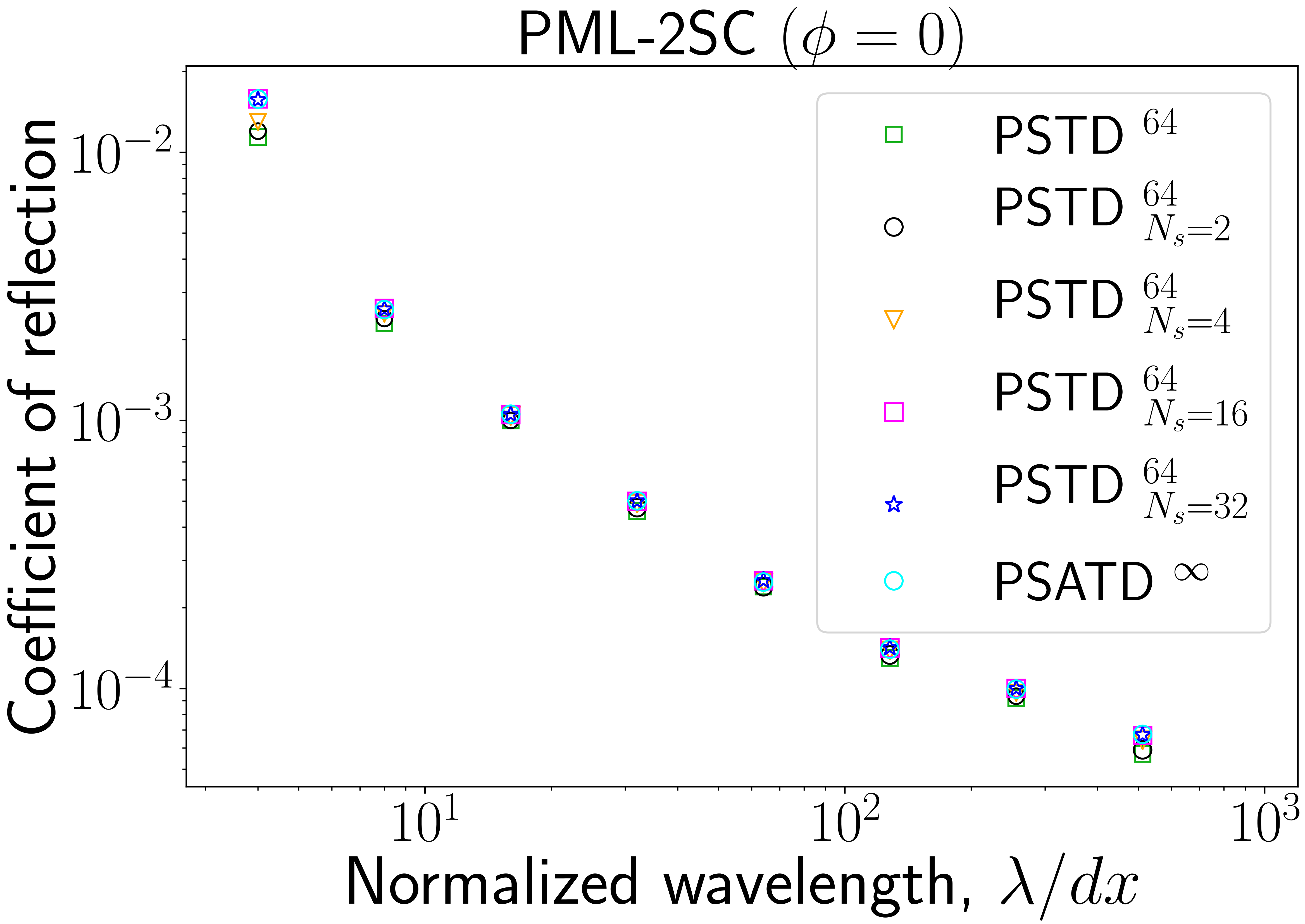


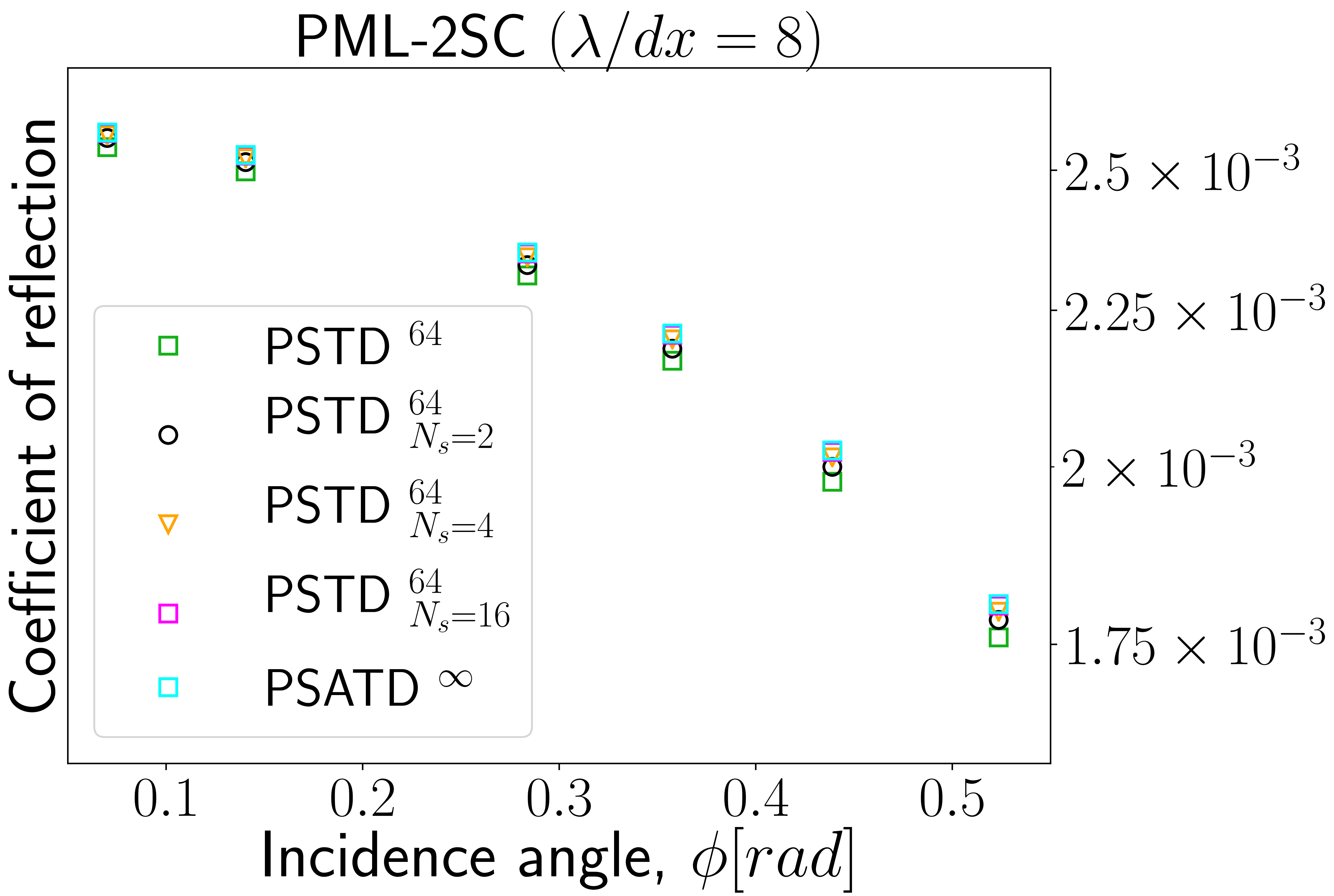
—— **theory ("p"-source model)**

△△△ **numerical calculation using PSTD^p**

PML-2SC: PSTD^{64}, PSTD$^{64}_{Ns}$ (N_S=2,8,16,32) AND PSATD$^{\infty}$

N_s is the order of sub-cycling in time (**N_s = m: Δt/m**)

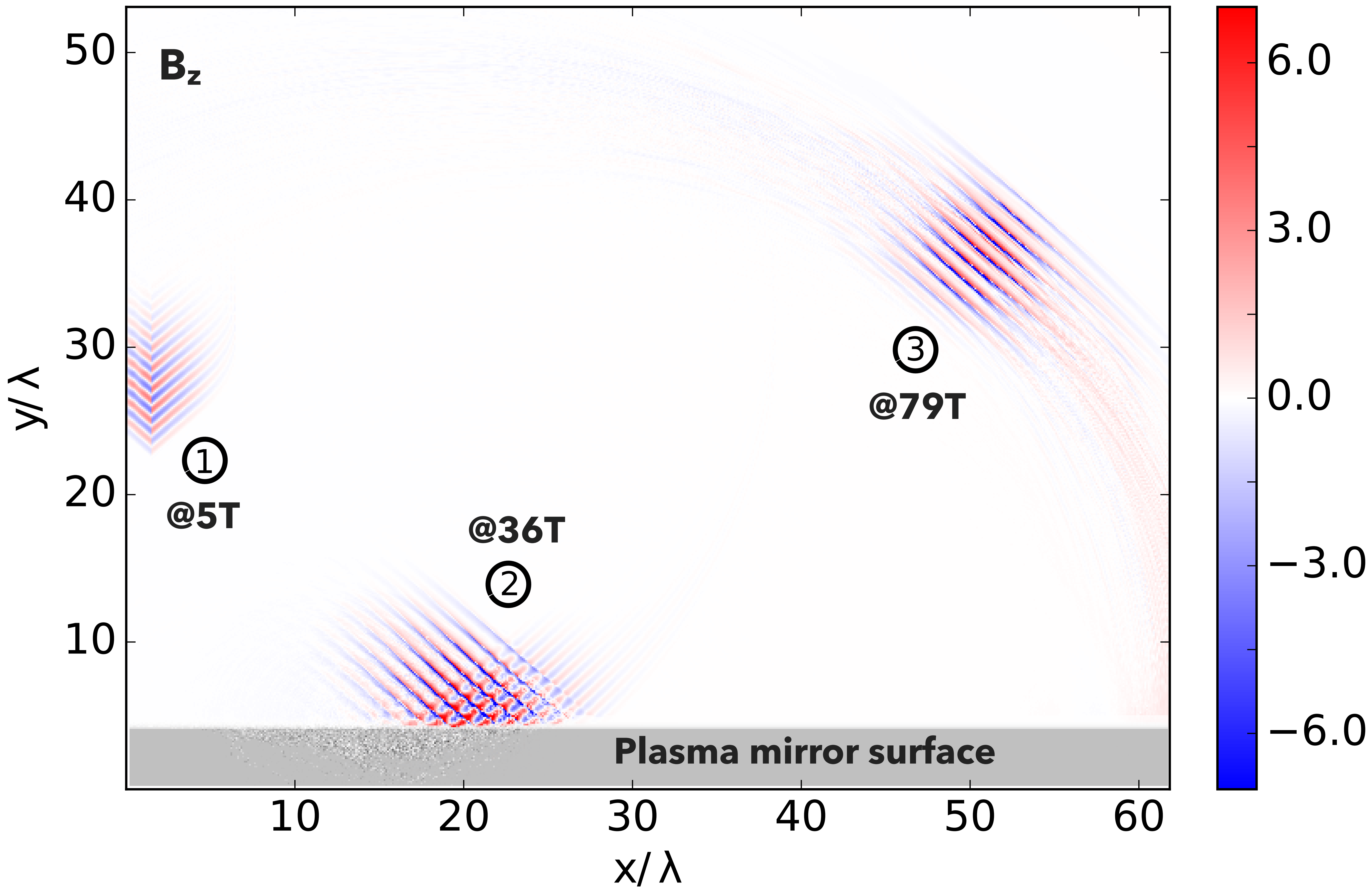




△△△ **numerical calculation using PSTD$^{p}_{Ns}$ or PSTD$^{\infty}$**

TEST OF THE NEW TWO-STEP FORMULATION IN LASER PLASMA EM-PIC SIMULATION

Simulation of 2D laser-plasma mirror interaction @ ultra-high intensity performed with **WARP+PXR** and the **new PML-2SC formulation**



1. Antenna radiates the laser field ☛ second "undesired field absorbed by left PML boundary w/o spurious reflection;
2. Laser field reflects from plasma mirror ☛ Harmonic generation in the reflected field
3. Reflected field approached right PML boundary ☛ well absorbed

T is the laser period

SUMMARY

- Novel "two-step" formulation has been introduced (starting from the standard FDTD then applying to arbitrary-order PSTD and PSATD solvers):
  - ✓Time-staggered "PML-2SS"
  - ✓Time centered "PML-2CS"
- Numerical dispersion analysis: PML-2SC's velocity and damping rates ~ standard (Berenger's) PML
- Simulation & analytical analysis: absorption rate of the PML-2SC's is preserved at any order of the solver, including at the limit of ∞ order, validating its applicability with PSATD Maxwell's solvers
- New PML formulation has been successfully implemented in a PIC code & applied to challenging modeling of plasma mirror

RESTRICTIONS AND FUTURE STUDIES

Study was restricted to the extension of the **split** formulation of the PML to PSATD. Further studies will examine the applicability to unspilt formulation (e.g., Uniaxial PML).

Thank you for your attention!

PSATD DISCRETIZATION

PSATD DISCRETIZATION

(under assumption that source terms are constant over one time interval
⇒ Maxwell's equation can be integrated analytically one time step)

$$
\begin{aligned}
H_{zx}|^{n+1}_{i+1/2,j+1/2} &= \mathcal{F}^{-1} C\Big(\mathcal{F} H_{zx}|^{n}_{i+1/2,j+1/2}\Big) - \Big(\mathcal{F}^{-1} iS\,\hat{k}_x e^{ik_x\Delta y/2}\Big(\mathcal{F} E_y|^{n}_{i+1/2,j+1/2}\Big)\Big),\\
H_{zy}|^{n+1}_{i+1/2,j+1/2} &= \mathcal{F}^{-1} C\Big(\mathcal{F} H_{zy}|^{n}_{i+1/2,j+1/2}\Big) + \Big(\mathcal{F}^{-1} iS\,\hat{k}_y e^{ik_y\Delta y/2}\Big(\mathcal{F} E_x|^{n}_{i+1/2,j+1/2}\Big)\Big),\\
E_x|^{n+1}_{i+1/2,j} &= \mathcal{F}^{-1} C\Big(\mathcal{F} E_x|^{n}_{i+1/2,j}\Big) + \Big(\mathcal{F}^{-1} iS\,\hat{k}_y e^{-ik_y\Delta y/2}\Big(\mathcal{F} H_z|^{n}_{i+1/2,j}\Big)\Big),\\
E_y|^{n+1}_{i,j+1/2} &= \mathcal{F}^{-1} C\Big(\mathcal{F} E_y|^{n}_{i,j+1/2}\Big) - \Big(\mathcal{F}^{-1} iS\,\hat{k}_x e^{-ik_x\Delta x/2}\Big(\mathcal{F} H_z|^{n}_{i,j+1/2}\Big)\Big),
\end{aligned}
$$

Spatial derivative in Fourier space:

$$\frac{\partial f(u)}{\partial u} = \frac{\partial}{\partial u}\int_{-\infty}^{\infty} \mathcal{F}[f(u)]e^{ik_u u}dk_u = \mathcal{F}^{-1} ik_u \mathcal{F}[f(u)]$$

$$[k_u]_p = \frac{2}{\Delta u}\sum_{l=1}^{p/2} c_l^p \sin\Big((2l-1)\frac{k_u\Delta u}{2}\Big),$$

$$
\begin{aligned}
\hat{\mathbf{k}} &= [\mathbf{k}]/k.\\
C &= \cos(\mathbf{k}c\Delta t)\\
S &= \sin(\mathbf{k}c\Delta t)
\end{aligned}
$$