Open boundary conditions for the envelope model in PIC simulations

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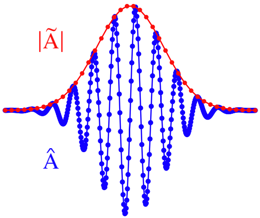
Time-averaged ponderomotive approximation



$$\hat{A}\left(\mathbf{r},t\right) = \mathbf{Re}\left[\tilde{A}(\mathbf{r},t)e^{ik_0(x-ct)}\right],$$

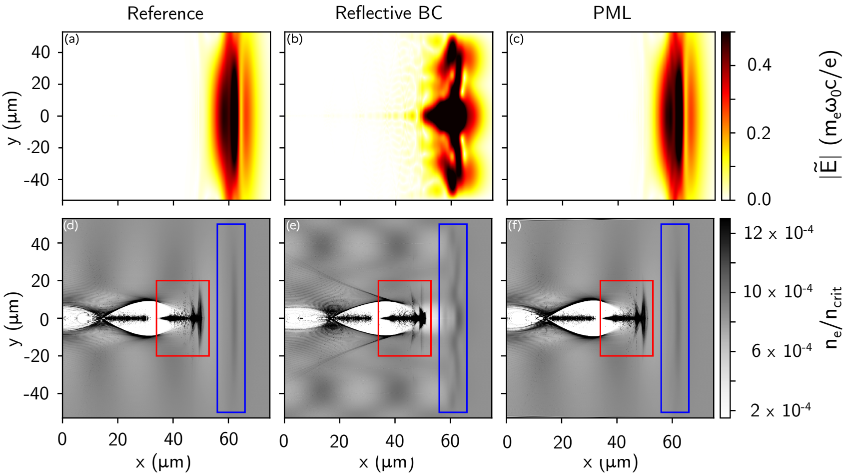
$$\nabla^2\tilde{A} + 2ik_0\left(\frac{\partial\tilde{A}}{\partial x} + \frac{1}{c}\frac{\partial\tilde{A}}{\partial t}\right) - \frac{1}{c^2}\frac{\partial^2\tilde{A}}{\partial t^2} = \chi\tilde{A}.$$

D. Terzani et al., Comp. Phys. Comm. **242**, 2019.

1. Important reduction of the simulation size and energy savings.
2. Mitigates numerical dispersion.
3. Easily parallelizable with an explicit scheme.
4. Lorentz invariant (see F. Massimo's talk)
5. Not suitable for all use cases.

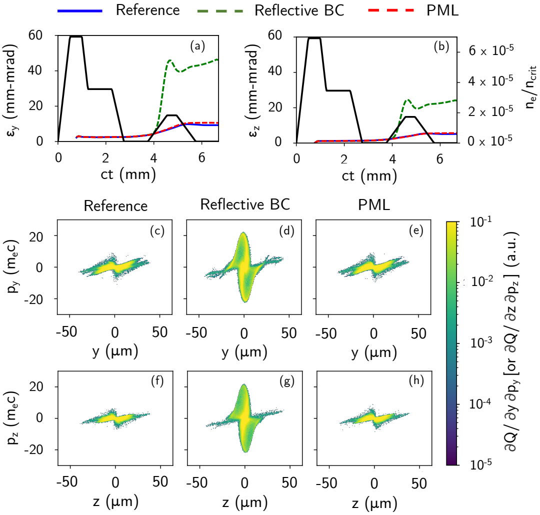
F. Massimo et al., Plasma Phys. Control. Fusion **67** 065032, 2025.

Open boundary conditions for LWFA simulations



G. Bouchard, et al., Comp. Phys. Comm. **315** 109737, 2025.

Open boundary conditions for LWFA simulations



G. Bouchard, et al., Comp. Phys. Comm. **315** 109737, 2025.

Credits

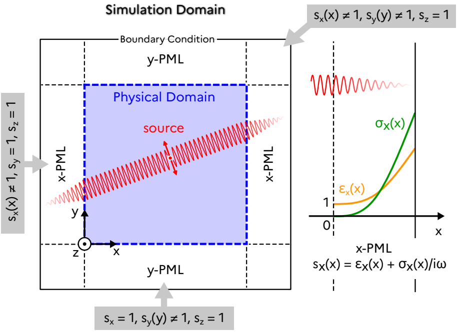
Main contribution by G. Bouchard.

CNRS,
Institut Polytechnique de Paris,
Paris-Saclay University.

F/OSS for electromagnetic PIC simulation.

Computational resources via the “Virtual Laplace” project.

Perfectly Matched Layers (PML)



- An extension of the physical domain.
- Damps traveling waves along the normal direction.
- Size defined by their number of cells (or layers).
- Properties defined by their local complex susceptibility.

Modified Maxwell's equations in a lossy media

For a monochromatic wave:

$$\boldsymbol{\nabla} \times \mathbf{H} = i\omega\epsilon_0[\varepsilon_r]\mathbf{E},$$

$$\boldsymbol{\nabla} \times \mathbf{E} = -i\omega\mu_0[\mu_r]\mathbf{H}.$$

$[\varepsilon_r]$ and $[\mu_r]$ are diagonal.

Vacuum matched impedance: $[\varepsilon_r] = [\mu_r] = [s]$.

C. A. Balanis. Advanced Engineering Electromagnetics. John Wiley & Sons, 2nd edition, 2011.

In a uniaxial PML along z reflections at the interface are prevented for all angles and frequencies:

$$[s]_z = \begin{pmatrix} s_z & 0 & 0 \\ 0 & s_z & 0 \\ 0 & 0 & s_z^{-1} \end{pmatrix}.$$

R. Lee, et al., *Perfectly matched anisotropic absorber for use as an absorbing boundary condition.* IEEE Transactions on Antennas and Propagation, 43, 1995.
S. D. Gedney. *An anisotropic pml absorbing media for the fdtd simulation of fields in lossy and dispersive media*. Electromagnetics, 16, 1996.

Modified Maxwell's equations in a lossy media

The **complex susceptibility** is written as:

$$s_z = \varepsilon_z + \frac{\sigma_z}{i\omega\varepsilon_0}.$$

Solutions are of the form:

$$E_y = E_0\, \mathrm{e}^{i(\omega\varepsilon_z t - k_z z)}\, \mathrm{e}^{\sigma_z t/\varepsilon_0}.$$

- Damping for all $\omega > 0$ if $\sigma_z < 0$.
- $\varepsilon_z > 1$ contributes to a better absorption of grazing waves.

But s_z is undefined when $\omega = 0$ and PML are unstable in certain conditions.

Modified envelope's equation in a lossy media

$$s_z = \varepsilon_z + \frac{\sigma_z}{i\omega\varepsilon_0}.$$

We apply a **frequency shift** (FS PML):

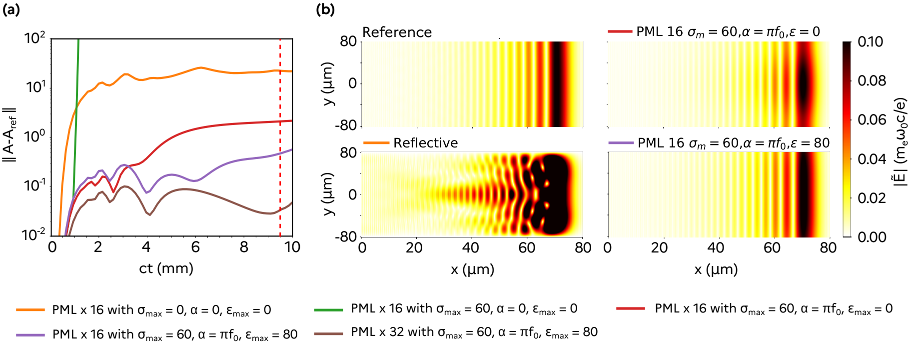
$$s_{z,fs} = \varepsilon_z + \frac{\sigma_z}{(\alpha_z + i\omega)\varepsilon_0} = \varepsilon_z + \frac{\alpha_z\sigma_z}{\epsilon_0(\alpha_z^2 + \omega^2)} + \frac{\frac{\omega^2}{\alpha_z^2+\omega^2}\sigma_z}{i\omega\varepsilon_0}.$$

M. Kuzuoglu, et al., IEEE Microwave and Guided Wave Letters, 6, 1996.

- A frequency dependent term is added to ε_z if $\alpha_z\sigma_z > 0$.
- Only frequencies $\omega > \alpha_z$ are properly damped.

A commonly chosen value for α_z is of the order of the lowest resolved angular frequency of the simulation $\alpha \sim 2\pi c/L_{sim}$.

The PML parameters effects



Why are PML sometimes unstable ?

- Surprisingly few theoretical constraints on $\sigma, \varepsilon, \alpha$.
- Empirical results show that they're better chosen monotonic, equal to vacuum properties at the interface and varying slowly.

The FDTD scheme may fail to resolve too strong local modifications and become unstable.

E. Becache, et al., *O*n the long-time behavior of unsplit perfectly matched layers, IEEE Trans. Antennas Propag. 52 (5), 2004.

A resonant terme at $-2k_0$ prevents stability of the longitudinal envelope PML if it propagates backwards.

PML envelope solver equation

$$
\begin{aligned}
\frac{1}{c^2}\frac{\partial^2 \tilde{A}}{\partial t^2} - 2ik_0\frac{1}{c}\frac{\partial \tilde{A}}{\partial t} = & \frac{\partial^2 \tilde{A}}{\partial x^2} + 2ik_0\frac{\partial \tilde{A}}{\partial x} + \frac{\partial^2 \tilde{A}}{\partial y^2} + \frac{\partial^2 \tilde{A}}{\partial z^2} \\
& + \big(\frac{1}{\varepsilon_y^2} - 1\big)\frac{\partial^2 \tilde{A}}{\partial y^2} - \frac{\varepsilon_y'}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y} \\
& + \frac{1}{p}\left(\frac{3\sigma_y\varepsilon_y' - \varepsilon_y\sigma_y'}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y} - \frac{2\sigma_y}{\varepsilon_y^2}\frac{\partial^2 \tilde{A}}{\partial y^2}\right) \\
& + \frac{1}{p^2}\left(\frac{2\varepsilon_y\sigma_y\sigma_y' + \varepsilon_y^2\sigma_y\alpha_y'\varepsilon_0 - 3\sigma_y^2\varepsilon_y'}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y} + \frac{\sigma_y^2}{\varepsilon_y^2}\frac{\partial^2 \tilde{A}}{\partial y^2}\right) \\
& + \frac{1}{p^3}\frac{\varepsilon_y'\sigma_y^3 - \varepsilon_y\sigma_y^2\sigma_y' - \varepsilon_y^2\sigma_y^2\alpha_y'\varepsilon_0}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y}, \\
& p = \varepsilon_y i\omega\varepsilon_0 + \varepsilon_y\alpha_y\varepsilon_0 + \sigma_y,
\end{aligned}
$$

Auxiliary differential equations

This equation can be solved explicitly with an FDTD scheme of this system of differential equations:

$$u_{0,y} = \left(\frac{1}{\varepsilon_y^2} - 1\right)\frac{\partial^2 \tilde{A}}{\partial y^2} - \frac{\varepsilon'_y}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y} + \tilde{u}_{1,y}, \qquad (1)$$

$$p\tilde{u}_{1,y} = \frac{3\sigma_y\varepsilon'_y - \varepsilon_y\sigma'_y}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y} - \frac{2\sigma_y}{\varepsilon_y^2}\frac{\partial^2 \tilde{A}}{\partial y^2} + \tilde{u}_{2,y}, \qquad (2)$$

$$p\tilde{u}_{2,y} = \frac{2\varepsilon_y\sigma_y\sigma'_y + \varepsilon_y^2\sigma_y\alpha'_y\varepsilon_0 - 3\sigma_y^2\varepsilon'_y}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y} + \frac{\sigma_y^2}{\varepsilon_y^2}\frac{\partial^2 \tilde{A}}{\partial y^2} + \tilde{u}_{3,y}, \qquad (3)$$

$$p\tilde{u}_{3,y} = \frac{\varepsilon'_y\sigma_y^3 - \varepsilon_y\sigma_y^2\sigma'_y - \varepsilon_y^2\sigma_y^2\alpha'_y\varepsilon_0}{\varepsilon_y^3}\frac{\partial \tilde{A}}{\partial y}. \qquad (4)$$

R. Martin, et al., Comput. Model. Eng. Sci. 56, 2010.
Y. Ma, et al., Ultrasonics 54 (6) 2014.

Conclusion

- A compromise between accuracy, stability and cost.
- A highly tunable implementation.
- Significantly widens the domain of application of the envelope model.
- Possible improvements regarding the longitudinal instability and the interface with non-vacuum.

Smilei)

https://smileipic.github.io/Smilei/

G. Bouchard, A. Beck, F. Massimo and A. Specka,
Perfectly Matched Layers implementation for E-H fields and complex wave envelope propagation in the Smilei PIC code
Comp. Phys. Comm. **315** 109737, 2025.

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